Quantum decimation renormalization group method for one dimensional spin-1/2 systems
by Chen Xiyao

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Physics
Montana State University
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Abstract:
We have extended both the reliability and the range of application of the decimation renormalization group method for calculating the thermal and magnetic properties of 1-dimensional quantum spin—1/2 systems. Efforts to improve the accuracy include increasing the spatial rescaling, investigating the effect of free versus periodic boundary conditions for each renormalization cluster and varying the iteration procedure. The systems under investigation include (1) spin chains with isotropic Heisenberg as well as Ising-like and XY-like anisotropic exchange in the presence of a longitudinal field, (2) chains with uniform antisymmetric exchange in a longitudinal field, (3) chains with alternating antiferromagnetic interactions in a field, and (4) those with anisotropic interactions in a field with arbitrary direction. The principal calculated results are magnetic and thermal response functions (susceptibility, magnetization and specific heat), which are compared (where possible) with previously published results using other techniques.
APPROVAL

of a thesis submitted by

Chen Xiyao

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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Apr 18, 1984
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ABSTRACT

We have extended both the reliability and the range of application of the decimation renormalization group method for calculating the thermal and magnetic properties of 1-dimensional quantum spin-1/2 systems. Efforts to improve the accuracy include increasing the spatial rescaling, investigating the effect of free versus periodic boundary conditions for each renormalization cluster and varying the iteration procedure. The systems under investigation include (1) spin chains with isotropic Heisenberg as well as Ising-like and XY-like anisotropic exchange in the presence of a longitudinal field, (2) chains with uniform antisymmetric exchange in a longitudinal field, (3) chains with alternating antiferromagnetic interactions in a field, and (4) those with anisotropic interactions in a field with arbitrary direction. The principal calculated results are magnetic and thermal response functions (susceptibility, magnetization and specific heat), which are compared (where possible) with previously published results using other techniques.
CHAPTER 1

INTRODUCTION

Interest in one-dimensional (1-D) magnetism arose in the early 1920's, and still continues to advance. A central reason for this is that 1-D models are, in general, more tractable than those in the familiar world of three dimensions. In fact there exist a number of exact solutions (as well as accurate approximate treatments) of a variety of 1-D problems, and an examination of these often illuminates the nature of the real physical systems. A second incentive is that experimentalists have found an increasing number of real magnetic systems whose structure is effectively one dimensional. Now essentially 1-D (quasi-1-D) magnets can be 'tailor-made' in the laboratory. Also popular is the field of organic conductors such as TTF-TCNQ, which are naturally quasi-1-D.

There exist several recent reviews of 1-D magnetic systems [1,2,3,4,5], detailing the current experimental and theoretical situations. For this reason the following discussion will briefly review only these developments which are important for the goals of this thesis.
Analytic Developments

The effective spin-1/2 Hamiltonian for the general anisotropic Heisenberg spin chain may be written in terms of Pauli spin operators as

\[ H = \sum_i ( -J_z \sigma_i^z \sigma_{i+1}^z - J_{xy}(\sigma_i^x \sigma_{i+1}^y - \sigma_i^y \sigma_{i+1}^x) - H_z \sigma_i^z - H_x \sigma_i^x \). \quad (1-1) \]

We consider bilinear spin couplings, and assume nearest-neighbor spin interactions only. The effective exchange constant between the Z-components of the spins is \( J_z \), and that between x and y components, \( J_{xy} \). The Ising model is obtained by putting \( J_{xy} = 0 \), and the XY-model is obtained by putting \( J_z = 0 \). If \( J = J_z = J_{xy} \) we have the isotropic Heisenberg chain.

The Ising model in the \( H_x = 0 \) case is purely classical, in the sense that all operators appearing in \( H \) commute with one another. This system was suggested by Lenz and solved in 1-D by Ising in 1925 [6]. The solution was essentially complete as a function of both temperature and applied magnetic field. This model has no phase transition at \( T > 0 \), but orders spontaneously at \( T = 0 \). In 1944, a very famous solution of the two-dimensional (2-D) Ising model was given by Onsager [7]. He found a transition at \( T > 0 \), but his solution provided information on the thermal properties in zero magnetic field alone. A complete solution, including \( H_z = 0 \), is lacking to this
Fully quantum-mechanical systems, such as the S=1/2 Heisenberg model are much more difficult to solve, even in 1-D. For the ferromagnetic case, J>0, the ground state consists of all spins parallel and is (N+1)-fold degenerate when H=0. In 1930 Bloch introduced the concept of a spin wave and gave the exact eigenstates for a single overturned spin. In 1963 the energy of the two-spin deviate state was obtained by Wortis [8], and Fukuda and Wortis [9], but the three- or more-spin deviate states are more difficult to get. For the antiferromagnetic case, J<0, Bethe in 1931 formulated an Ansatz concerning the general structure of the eigenstates, and found the ground-state eigenfunction for the S=1/2 Heisenberg antiferromagnetic chain. In doing so, he demonstrated that no long-range order exists in this model even at T=0 [10]. We note that the Bethe Ansatz remains the key to the analytic solutions of a wide class of spin chain models as well as a variety of 1- and 2-D systems other than quantum spin chains. In 1938 Hulthen derived the ground-state energy for this antiferromagnetic model [11]:

\[ E = -N|J|(21n2-1/2) = -0.886N|J| \]

as compared with \(-0.5N|J|\) for classical Néel antiferromagnetic ground state. Not until 1962 did des Cloizeaux and Pearson derive the energy spectrum of the
lowest excited triplet states, finding the dispersion relation to be [12]:
\[ \hbar \omega(q) = \pi |J \sin qa| \]
where \( a \) is the separation between nearest-neighbor atoms along the chain.

The 1-D spin-1/2 XY model was solved analytically in the 1960's independently by Lieb, Schultz and Mattis [13] and Katsura [14]. Katsura [14] and Pfeuty [15] also obtained exact results for the Ising model in a transverse magnetic field, often described as the simplest solvable quantum mechanical model.

Real progress on the general spin-1/2 Ising-Heisenberg-XY linear chain with symmetry in the XY plane, dates from 1966 and the work of Yang and Yang, who obtained a detailed zero temperature solution in terms of anisotropy and magnetic field [16]. In 1980 Johnson and Bonner found the elementary excitations and low-temperature thermodynamics for the Ising-Heisenberg ferromagnet in zero and very small magnetic field [17]. A complete solution of this model has yet to be obtained.

**Numerical Studies**

As indicated above, a complete analytic solution for the \( S=1/2 \) general anisotropic Heisenberg linear chain is not available even now. For the \( S>1/2 \) spin chain an analytic treatment along the lines of the Bethe Ansatz may be not possible. There is experimental interest in a
variety of $S > 1/2$ spin chains, such as effective spin-1 system (containing the Ni$^{2+}$ ion), spin-3/2 system (Cr$^{3+}$ ion), and spin-5/2 system (Mn$^{2+}$ ion). Even for spin 1/2, the Bethe Ansatz approach cannot be applied to the Heisenberg alternating chain, whose Hamiltonian can be written as

$$\mathcal{H} = -\sum_{i} \left( J_{1}\sigma_{2i-1}\sigma_{2i} + J_{2}\sigma_{2i}\sigma_{2i+1} \right).$$  \hspace{1cm} (1-2)$$

This is a nearest-neighbor exchange model in which there are two unequal exchange constants, $|J_{1}| > |J_{2}|$ say. It is convenient to define an alternation ratio $\alpha = J_{2}/J_{1}$, so that $\alpha = 1$ corresponds to the uniform limit and $\alpha = 0$ corresponds to the case of decoupled dimers. The alternating spin chain is important as well to the theory of spin-Peierls transitions in quasi-1-D organics. Since an analytic approach is not feasible at this time, other reliable theoretical calculations are needed.

In the 1960's Bonner and Fisher [18] and, independently, Griffiths [19] developed a technique referred to as finite chain extrapolation. This involves calculating exactly the properties of a sequence of small finite spin chains, with both periodic and free-end boundary conditions, and steadily increasing the system size $N$. Numerical extrapolations are then made to the thermodynamic limit ($N \rightarrow \infty$). In this way an
extensive set of results for all $H$ and $T$, and some results for the $T=0$ correlation functions were obtained for the uniform chain with accuracy comparable to experiment [18]. By the same procedure, Blöte obtained the ground-state energies [20], specific heat [21], susceptibility, and $T=0$ magnetization isotherms vs. field [22] for spin values $S=1/2, 1, 3/2, 2$, up to $5/2$. Diederix, Blöte et al. compared the experimental and the calculated thermodynamic properties for 1-D alternating Heisenberg antiferromagnet chain in copper nitrate $\text{Cu(NO}_3\text{)}_2\cdot2.5\text{H}_2\text{O}$ [23].

**Real Space Renormalization Group and Quantum Renormalization Group (QRG)**

The renormalization group approach [24] is the most powerful and successful method in the modern theory of critical phenomena, but its use has been confined mainly to classical systems. For example, the real space renormalization group method pioneered by Niemeijer and van Leeuwen [25] has been successfully applied to Ising models [26,27], while momentum-space techniques have been widely used in studying models in which the spins are classical $n$-dimensional vectors [28]. However, classical spins have their limitations as models for magnetic phenomena, since magnetic systems have a quantum nature that cannot be ignored [29], especially at very low temperature and in low dimensions. Considerably greater difficulty, however, is experienced in applying
RG methods to quantum mechanical systems. The essential reason is the familiar problem of noncommuting operators.

Very recently two kinds of RG methods have been tested on quantum models. One is the block transformation method devised first by field theorists [30,31] and shortly thereafter applied to a type of Kondo problem [32]. Most block RG approaches have been used for T=0 cases, and only a very few for T>0 [33,34,35].

The spirit of the block RG is as follows. The lattice is subdivided into blocks of $N_s$ sites such that the eigenvalues and eigenvectors of each block may be calculated exactly. The basis of each block (2$N_s$ levels, $S=1/2$) is truncated to some number $N_1$ of levels, and the coupling between the blocks is written within the truncated basis. For T=0 cases, the truncated basis need only contain the ground state and dominant set of first excited states.

This block QRG method has been exhaustively tested on the transverse Ising model, with encouraging results [30,36]. Fields et al. [37,38,39] used a T=0 approach on the 1-D alternating Heisenberg antiferromagnet chain in order to investigate the nature of the lowest excited state as a function of alternation ratio $\alpha$. The block QRG calculations fall naturally into two classes: $N_s$ odd, (3, 5, 7 and 9), with $N_1=2$ and $N_s$ even, with $N_1=4$ (or 6 or 8). The $N_s$ odd calculation means that one $N_s$-spin
block maps into one renormalized site. The $N_s$ even
calculation means that the $N_s$-spin block maps into a
renormalized $N_1/2$-spin block. Fields et al. used the $N_s$ odd
method and found that the uniform limit ($\alpha=1$) is always an
unstable fixed point of system, while a system of
independent dimers ($\alpha=0$) is a stable fixed point. Therefore
this $T=0$ QRG predicts an excitation gap that vanishes only
in the uniform limit (no alternation). They also examined
the quantitative accuracy of this QRG by comparing with
finite chain extrapolation results. For the ground-state
energy, the $N_1=2$, $N_s=9$ RG calculation gives a quantitative
discrepancy amounting to 12% in the uniform limit. However,
the $N_1=2$ RG sequence, $N_s = 3, 5, 7$ and 9, extrapolated to
$N_s=\infty$, gives more accurate results. For the excitation gap,
the $N_s$ odd calculation gives a value that is quantitatively
unreliable near the dimer limit. The $N_s$ even calculation
gives results in very good agreement with the extrapolated
curve out to $\alpha=0.6$ but predicts a gap vanishing at $\alpha=0.962$
rather than unity.

The second QRG method is the decimation
transformation method first extended by Suzuki and Takano
from its classical version [40,41,42,43]. This seems to be
the simplest RG approach for quantum spin systems. As
reviewed in detail below, Suzuki et al. calculated the
temperature dependence of the internal energy and specific
heat of the uniform 1-D spin models (the isotropic
Heisenberg model with ferro- and antiferromagnetic couplings, and XY-model).

In this thesis we will be concerned exclusively with the decimation RG. Unlike the block method, it can be readily applied at finite temperature and in a magnetic field. Furthermore the decimation approach is correct in both the dimer and Ising limits.

The purpose of this thesis is to extend both the reliability and the range of application of the decimation method. We attempt to improve its accuracy by increasing the length rescaling factor and investigating the effect of boundary conditions.

We apply decimation to the calculation of thermodynamic properties by various iteration techniques. In particular we examine the thermal and magnetic behavior of (1) uniform anisotropic Heisenberg chains, (2) uniform, anisotropic Heisenberg chains with antisymmetric exchange, and (3) alternating anisotropic Heisenberg chains. Finally, we extend this QRG to anisotropic spin chains in a magnetic field with arbitrary direction. Wherever possible, we have compared our results with those of other techniques.
Suzuki and Takano (ST) have proposed a simple decimation RG transformation for 1-D quantum spin systems \([40,41]\), with nearest-neighbor interactions only. In this section we illustrate the method by reviewing the ST treatment of the spin-1/2 Heisenberg model with uniaxial anisotropy. The reduced Hamiltonian \((-\text{energy}/k_BT)\) of this model is given by

\[
\tilde{\mathcal{H}} = \sum_{i=0}^{N-1} \left\{ K_z \sigma_i^z \sigma_{i+1}^z + K_{xy} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) \right\}, \quad (2-1)
\]

where \(T\) is the temperature and \(k_B\) Boltzmann's constant. Here \(\sigma_i^x, \sigma_i^y, \text{ and } \sigma_i^z\) denote the Pauli spin operators on the \(i\)th site of the linear chain with \(N\) sites. The parameters \(K_z\) and \(K_{xy}\) are respectively \(-\beta J_z\) and \(-\beta J_{xy}\), where \(J_z\) is the exchange coupling constant between \(z\) components of neighboring spins, \(J_{xy}\) is that between \(x\) and \(y\) components, and \(\beta = 1/k_BT\).

We construct a decimation transformation with scale factor \(L\) (see Fig. 1) according to the procedure

\[
\exp\{ A + \tilde{\mathcal{H}} \} = \text{Tr}' \exp\{ \tilde{\mathcal{H}} \}. \quad (2-2)
\]
Here $\tilde{\mathcal{H}}$ is Hamiltonian on the original lattice (2-1) and $\tilde{\mathcal{H}}'$ is a decimated (i.e. renormalized) Hamiltonian on the new lattice with lattice spacing $L_a$, (where $a$ is lattice spacing of original chain). The operation $\text{Tr}'$ means to take a partial trace over all spin operators except those belonging to the new lattice.

Fig. 1. Decimation in one dimension with scale factor $L=2$. Crosses denote spin operators to be eliminated (traced over) by the decimation. Dots denote spin operators to remain after the decimation. Lines denote the interactions between neighboring spins.
For a 1-D classical system, say the Ising model, this decimation can be carried out exactly. However, in the quantum case it is impossible to carry out the decimation exactly even in one dimension because of the noncommuting effect of operators in the Hamiltonian. ST have proposed the following simple approximation for the one-dimensional decimation.

First the full Hamiltonian is divided into a sum of cluster Hamiltonians $H_{bj}$:

$$\hat{\mathcal{H}} = \sum_{j=1}^{N/L} H_{bj}. \quad (2-3)$$

Here

$$H_{bj} = \sum_{i=1}^{L} H(\sigma_{j,i-1},\sigma_{j,i}),$$

where $H(\sigma_{j,i-1},\sigma_{j,i})$ denotes a nearest-neighbor interaction between $\sigma_{i-1}$ and $\sigma_{i}$ in the $j$th cluster. We then ignore the commutators between operators referred to different clusters, and make the exact decimation within one cluster only:

$$\exp\{ A_1 + H_{b'}(\sigma_0,\sigma_L) \} = \text{Tr} \exp\{ H_{b}(\sigma_0,\sigma_1,\ldots,\sigma_L) \}. \quad (2-4)$$

$H_{b'}(\sigma_0,\sigma_L)$ is a renormalized nearest-neighbor interaction between the remaining spins $\sigma_0$ and $\sigma_L$, and $A_1$
is a constant term independent of $\sigma_0$ and $\sigma_L$. Then, using $H_{bj'}$ and $A_1$, we construct an approximate transformed Hamiltonian $\tilde{\mathcal{H}}_a$ and an approximate constant term $A_a$ as follows:

$$\frac{N}{L} \sum_{j=1}^{N/L} H_{bj'}(\sigma_j,0,\sigma_j,L), \quad (2-5)$$

and

$$A_a = (N/L) A_1.$$

This entire procedure (see Fig. 2) can be written as

$$\exp\{A + \frac{N}{L} \mathcal{H}_a'\} = \exp\{H_{bj'}\} \exp\{H_{bj}\} \exp\{A_1 + H_{bj'}\} \approx \exp\{NA_1/L + \sum_{j=1}^{N/L} H_{bj'}\} = \exp\{A + \frac{N}{L} \mathcal{H}_a'\}. \quad (2-6)$$

Two approximations have been made, and both introduce errors due to the non-commutativity of operators. Their nature can be examined by considering the case of two adjacent clusters only, for which we may write

$$\exp\{H_{b1} + H_{b2}\} = \exp\{H_{b1}\} \exp\{H_{b2}\} \exp\{1/2 [H_{b1},H_{b2}] + \cdots\}$$

$$\exp\{H_{b1'}\} \exp\{H_{b2'}\} = \exp\{H_{b1'} + H_{b2'} - 1/2 [H_{b1'},H_{b2'}] + \cdots\} \quad (2-7)$$
Roughly speaking, the errors which are introduced in truncating these expressions have opposite signs. Consequently they may be expected to cancel, at least, in part, since $H_b$ is transformed into $H_b'$ in (2-7) after the decimation.

Fig. 2. The approximate one-dimensional decimation. The original system is divided into a sum of clusters in (a). The decimation is carried out within one cluster shown in (b), to give a new interaction which is denoted by a wave line in (c). From this new interaction, the renormalized system (d) is constructed.
Applying the approximation explained above to the Hamiltonian (2-1) we can carry out the decimation with $L=2$. The Hamiltonian of one cluster is

$$H_b = K_z(\sigma_0 z \sigma_1 z + \sigma_1 z \sigma_2 z) + K_{xy}(\sigma_0 x \sigma_1 x + \sigma_1 x \sigma_2 x + \sigma_0 y \sigma_1 y + \sigma_1 y \sigma_2 y).$$

$$= K_z(\sigma_0 z \sigma_1 z + \sigma_1 z \sigma_2 z) + K_{xy}/2(\sigma_0^+ \sigma_1^- + \sigma_1^+ \sigma_2^- + \text{h.c.}).$$

(2-8)

Here h.c means Hermitian conjugate and

$$\sigma^+ = \sigma x + i \sigma y \quad \text{and} \quad \sigma^- = \sigma x - i \sigma y.$$

(2-9)

The eigenstates $|m\rangle$ and the eigenvalues $E_m$ of the Hamiltonian $H_b$ can be obtained analytically (see Table 1) for the cluster of $L+1=3$ sites. The transformed Hamiltonian $H'_b$ is of the same form as Eq. (2-8), e.g.

$$H'_b = K'_z \sigma_0^2 \sigma_2^z + K_{xy}'/2(\sigma_0^+ \sigma_2^- + \sigma_0^- \sigma_2^+).$$

It has eigenstates $|n\rangle$ and eigenvalues $E_n'$ (see Table 2). The decimation Eq. (2-4) can be written in the form

$$\exp\{A_1\} \sum_{\{n\}} \exp\{E_n'\} |n\rangle\langle n| = \text{Tr}' \sum_{\{m\}} \exp\{E_m\} |m\rangle\langle m| =$$

$$= \sum_{\{m,i\}} \langle i|m\rangle\langle m|i \rangle \exp\{E_m\},$$

(2-10)

where $|i\rangle$'s are all states of the $L-1=1$ intermediate sites.
Table 1. The eight eigenstates and eigenvalues of a three spin cluster

| m | $|m\rangle$ | $E_m$ |
|---|---|---|
| 1 | $|\uparrow\uparrow\uparrow\rangle$ | $2K_z$ |
| 2 | $|\downarrow\downarrow\downarrow\rangle$ | $2K_z$ |
| 3 | $a_+ |\uparrow\downarrow\downarrow + \downarrow\uparrow\uparrow\rangle + b_+ |\uparrow\uparrow\uparrow\rangle$ | $E_+ = -K_z + G$ |
| 4 | $a_- |\uparrow\downarrow\downarrow + \downarrow\uparrow\uparrow\rangle + b_- |\uparrow\uparrow\uparrow\rangle$ | $E_- = -K_z - G$ |
| 5 | $a_+ |\downarrow\uparrow\downarrow + \uparrow\downarrow\uparrow\rangle + b_+ |\downarrow\uparrow\uparrow\rangle$ | $E_+ = -K_z + G$ |
| 6 | $a_- |\downarrow\uparrow\downarrow + \uparrow\downarrow\uparrow\rangle + b_- |\downarrow\uparrow\uparrow\rangle$ | $E_- = -K_z - G$ |
| 7 | $1/\sqrt{2} |\uparrow\downarrow\downarrow - \downarrow\uparrow\uparrow\rangle$ | 0 |
| 8 | $1/\sqrt{2} |\downarrow\uparrow\downarrow - \uparrow\downarrow\uparrow\rangle$ | 0 |

* $G^2 = K_z^2 + 8K_{xy}^2$

$$a_{+2} = 4K_{xy}^2/(8K_{xy}^2 + E_{+2})$$
$$a_{-2} = 4K_{xy}^2/(8K_{xy}^2 + E_{-2})$$
$$b_{+2} = E_{+2}/(8K_{xy}^2 + E_{+2})$$
$$b_{-2} = E_{-2}/(8K_{xy}^2 + E_{-2})$$

Table 2. The four eigenstates and eigenvalues of a two spin cluster

| n | $|n\rangle$ | $E_n$ |
|---|---|---|
| 1 | $|\uparrow\uparrow\rangle$ | $K_z$ |
| 2 | $|\downarrow\downarrow\rangle$ | $K_z$ |
| 3 | $1/\sqrt{2} |\uparrow\downarrow + \downarrow\uparrow\rangle$ | $-K_z + 2K_{xy}$ |
| 4 | $1/\sqrt{2} |\uparrow\downarrow - \downarrow\uparrow\rangle$ | $-K_z - 2K_{xy}$ |
Substituting these eigenstates and eigenvalues in the Table 1 and 2 into Eq.(2-10), we thus obtain

\[
\begin{align*}
A_1 + K_z' &= \ln\{ \exp(2K_z) + b_+^2\exp(E_+) + b_-^2\exp(E_-) \} \\
A_1 - K_z' + 2K_{xy}' &= \ln 4 + \ln\{ a_+^2\exp(E_+) + a_-^2\exp(E_-) \} \\
A_1 - K_z' - 2K_{xy}' &= \ln 2
\end{align*}
\]

Therefore we find the parameters in the transformed Hamiltonian \( H'_b \):  
\[
\begin{align*}
K_{xy}' &= \frac{1}{4} \ln\{ \exp(-K_z) (\cosh G + K_z/G \sinh G) \} \\
K_z' &= \frac{1}{2} \ln\{ \exp(2K_z) + \exp(-K_z) (\cosh G - K_z/G \sinh G) \} \\
&\quad - \frac{1}{2} \ln 2 - K_{xy}' \\
A_1 &= K_z' + 2K_{xy}' + \ln 2
\end{align*}
\]

For this example ST also calculated the magnitude of the error involved in this approximation:

\[
\Delta K_z' \sim \Delta K_{xy}' \sim \Delta A_1 \sim O(K^4)
\]

These results show that the effects of noncommutativity neglected in the approximations start at the fourth order in \( K_z \) and \( K_{xy} \). Thus, the approximation becomes better at higher temperature. Thermodynamic properties are calculated by iterating the renormalization transformations, as will be discussed below. The thermodynamic properties obtained from this approximation are found at high temperature to be in good agreement with those found by Bonner and Fisher and by Katsura.
2.2 SPIN CHAINS IN A LONGITUDINAL FIELD

The approximate quantum decimation is summarized in Eq. (2-6). In this section and the next we will use this method to examine a variety of spin systems. We will also investigate the effects of increasing the scale factor, of using periodic rather than free boundary conditions for each cluster, and by varying the iteration procedure which is used to calculate the thermodynamic properties. The outline of the remainder of this chapter is as follows: In this section, we study the 1-D model with both symmetric and antisymmetric exchange, as well as alternating antiferromagnetic spin chain. The effects of scale factors, boundary conditions, and iteration methods will be tested in the alternating spin chain. In next section, a general decimation method for spin chains in a magnetic field of arbitrary direction is studied.

2.2.1 Antisymmetric Exchange

Antisymmetric, or Dzyaloshinskii-Moriya (DM) interactions [44,45] are of the form \( \vec{D} \cdot (\vec{S}_i \times \vec{S}_j) \), where \( \vec{D} \) is a three-component interaction constant and \( \vec{S}_i \) and \( \vec{S}_j \) are spins on chain sites i and j. Terms of this type may arise due to spin-orbit coupling in low-symmetry magnetic structures. Among those materials in which DM interactions have been commonly observed are low-dimensional Jahn-Teller distorted compounds. Another recent example is the
chain-like polymer poly (cobalt n-butylphosphinate)[46], in which the symmetric interaction (that is \( S_i \cdot S_j \)) is isotropic and antiferromagnetic, while the DM term produces weak ferromagnetism. In a given system DM interactions are typically an order of magnitude weaker than the symmetric \((S \cdot S)\) coupling. Nonetheless their effects on the response functions may be significant, and are known in detail only via series expansions [47] valid in the high temperature regime.

Betts has pointed out that if \( \vec{D}_{ij} \) points in the same direction for all pairs of nearest neighbors, and if the lattice is one which can be divided into sublattices, a DM interaction can be transformed into an XY interaction by rotating the axes for spins on one sublattice through 90° about the direction of \( \vec{D} \). If there is also a symmetrical (Heisenberg or XY) interaction between the spins, a rotation through \( \tan^{-1}(|\vec{D}|/J) \) about \( \vec{D} \) would eliminate the antisymmetric part of the interaction [47,48].

In the case that there is an isotropy in the XY-plane, that is where the antisymmetric exchange constant has only a Z component, \( D = D_z \), and that the applied field is in the same direction, the Betts's statement gives the following mapping relation: The Hamiltonian of the spin chain with antisymmetric exchange
\[ \mathcal{H} = \sum_i \{ -K_z S_i^z S_{i+1}^z - K_{xy} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - \\
- D (S_i^x S_{i+1}^y - S_i^y S_{i+1}^x) - \hbar S_i^z \} \] (2-12)

is in fact equivalent to an anisotropic spin chain with Hamiltonian

\[ \mathcal{H} = \sum_i \{ -K_z S_i^z S_{i+1}^z - K_{xy}' (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - \hbar S_i^z \} \] (2-13)

where

\[ K_{xy}' = \sqrt{K_{xy}^2 + D^2} \] (2-14)

This can be proved as follows:

In the Hamiltonian (2-12) one rotates the successive \( S_i \) about the \( Z \) axis, using

\[
\begin{align*}
S_{i+1}^x &= \cos \Delta S_i^x S_{i+1}^{x'} - \sin \Delta S_i^y S_{i+1}^{y'} \\
S_{i+1}^y &= \sin \Delta S_i^x S_{i+1}^{x'} + \cos \Delta S_i^y S_{i+1}^{y'} \\
S_{i+1}^z &= S_i^z
\end{align*}
\] (2-15)

If we fix \( \Delta \) by the relation

\[ \tan \Delta = \frac{D}{K_{xy}} \] (2-16)

substituting Eq. (2-15) and (2-16) into Hamiltonian (2-12) gives

\[ \mathcal{H} = \sum_i \{ -K_z S_i^z S_{i+1}^z - \sqrt{K_{xy}^2 + D^2} (S_i^x S_{i+1}^{x'} + S_i^y S_{i+1}^{y'}) - \\
- \hbar S_i^z \} \] (2-17)
Comparing Eq.(2-13) with Eq.(2-17), we have Eq.(2-14).

Both antisymmetric and symmetric exchanges are isotropic in the XY-plane. In the above we see that if a suitable rotation is made in the XY-plane, the antisymmetric exchange is changed into a symmetric one. If there exists a transverse field (i.e., in the XY-plane), the isotropy in the XY-plane is broken. Thus the mapping to a symmetric exchange holds only for the longitudinal field case.

In this subsection we test whether the QRG method, with its uncontrolled approximations, can treat the additional complexity of antisymmetric exchange. We will calculate the specific heat of the Heisenberg chain by the decimation RG, and check that we reproduce the same results as with anisotropic symmetric exchange.

The reduced Hamiltonian for this case is

$$\tilde{H} = \sum_i \left[ -Kz_\sigma i \sigma_{i+1} - K_{xy} (\sigma_i x \sigma_{i+1} x + \sigma_i y \sigma_{i+1} y) - D(\sigma_i x \sigma_{i+1} y - \sigma_i y \sigma_{i+1} x) - h (\sigma_i z) \right], \quad (2-18)$$

Here $\sigma = 2z$, $K_z = \beta J_z$, $K_{xy} = \beta J_{xy}$, $h = \beta H_z$, and $\beta = 1/kBT$.

We use decimation with scale factor $L=2$ to calculate the thermodynamic properties. The Hamiltonian of a three spin cluster is

$$\tilde{H}_b = -K_z (\sigma_0^z \sigma_1^z + \sigma_1^z \sigma_2^z) - 1/2 (K_{xy} + iD) (\sigma_0^+ \sigma_1^- + \sigma_1^+ \sigma_2^-) - 1/2 (K_{xy} - iD) (\sigma_0^- \sigma_1^+ + \sigma_1^- \sigma_2^+) - h (\sigma_0^z / 2 + \sigma_1^z + \sigma_2^z / 2). \quad (2-19)$$
We have used Eq. (2-9) to write

\[ \sigma_1 x \sigma_2 y - \sigma_1 y \sigma_2 x = i/2 \left( \sigma_1^+ \sigma_2^- - \sigma_1^- \sigma_2^+ \right) , \]

and take account the fact that since each end spin is shared by two neighboring clusters, half the Zeeman term should be included with each cluster. This Hamiltonian commutes with the Z component of the total spin. Therefore we can easily solve for its eigenstates and eigenvalues analytically, as shown in Table 3a. The transformed Hamiltonian \( H_b' \) is of the same form as Eq. (2-19), but for a two-spin cluster:

\[ H_b' = -K_z' \sigma_0^z \sigma_2^z - 1/2(K_{xy'} + iD') \sigma_0^- \sigma_2^+ - 1/2(K_{xy'} - iD') \sigma_0^+ \sigma_2^- - \hbar'/2 \left( \sigma_0^z + \sigma_2^z \right) . \]

Its eigenstates and eigenvalues are shown in Table 3b.

Substituting these eigenstates and eigenvalues in the Table 3a and 3b into Eq. (2-10) (but changing the sign of the energy), we also require that

\[ a = d \quad (2-20) \]

to keep the two spin eigenstates consistent with those arising from the decimation. Therefore we find

\[ \exp\{\Lambda_1 - H_b'\} = \sum_{n=1}^{4} |n><n| \exp\{-E_n'\} = \sum_{n=1}^{4} |n><n| P_n . \quad (2-21) \]
Table 3a. Eigenstates and eigenvalues of a three spin cluster with antisymmetric exchange

| $m$ | $| m \rangle$ | $E_m$ |
|-----|----------------|------|
| 1   | $| \uparrow \uparrow \uparrow \rangle$ | $-2K_z - 2h$ |
| 2   | $| \downarrow \downarrow \downarrow \rangle$ | $-2K_z + 2h$ |
| 3   | $1/\sqrt{2} (| \uparrow \uparrow \downarrow \rangle - a | \uparrow \uparrow \uparrow \rangle)$ | $-h$ |
| 4   | $1/\sqrt{2} (| \uparrow \downarrow \uparrow \rangle - a^* | \uparrow \uparrow \uparrow \rangle)$ | $h$ |
| 5   | $1/\sqrt{1+2|b_+|^2} | b_+ \uparrow \uparrow \uparrow + \uparrow \uparrow \uparrow + b_+^* \downarrow \downarrow \downarrow \rangle$ | $E_{1+}$ |
| 6   | $1/\sqrt{1+2|b_-|^2} | b_- \uparrow \uparrow \uparrow + \uparrow \uparrow \uparrow + b_-^* \downarrow \downarrow \downarrow \rangle$ | $E_{1-}$ |
| 7   | $1/\sqrt{1+2|c_+|^2} | c_+ \uparrow \downarrow \uparrow + \uparrow \uparrow \uparrow + c_+^* \downarrow \downarrow \downarrow \rangle$ | $E_{2+}$ |
| 8   | $1/\sqrt{1+2|c_-|^2} | c_- \uparrow \downarrow \uparrow + \uparrow \uparrow \uparrow + c_-^* \downarrow \downarrow \downarrow \rangle$ | $E_{2-}$ |

$a = (K_{xy} - iD)^2 / (K_{xy}^2 + D^2)$

$b_+ = -2(K_{xy} + iD) / (h + E_{1+})$

$b_- = -2(K_{xy} + iD) / (h + E_{1-})$

$c_+ = 2(K_{xy} - iD) / (h - E_{2+})$

$c_- = 2(K_{xy} - iD) / (h - E_{2-})$

$E_{1+} = -h/2 + K_z + \sqrt{8(K_{xy}^2 + D^2) + (h/2 + K_z)^2}$

$E_{1-} = -h/2 + K_z - \sqrt{8(K_{xy}^2 + D^2) + (h/2 + K_z)^2}$

$E_{2+} = h/2 + K_z + \sqrt{8(K_{xy}^2 + D^2) + (-h/2 + K_z)^2}$

$E_{2-} = h/2 + K_z - \sqrt{8(K_{xy}^2 + D^2) + (-h/2 + K_z)^2}$
Table 3b. The four eigenstates and eigenvalues of a two spin cluster with antisymmetric exchange

<table>
<thead>
<tr>
<th>n</th>
<th>( E_n' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>1\rangle ) = (</td>
</tr>
<tr>
<td>(</td>
<td>2\rangle ) = (</td>
</tr>
<tr>
<td>(</td>
<td>3\rangle ) = ( 1/\sqrt{2}</td>
</tr>
<tr>
<td>(</td>
<td>4\rangle ) = ( 1/\sqrt{2}</td>
</tr>
</tbody>
</table>

where

\[
\begin{align*}
    P_1 &= \exp(2K_z + 2h) + 1/(1+2|b_+|^2) \exp(-E_{1+}) + \\
        &\quad + 1/(1+2|b_-|^2) \exp(-E_{1-}) \\
    P_2 &= \exp(2K_z - 2h) + 1/(1+2|c_+|^2) \exp(-E_{2+}) + \\
        &\quad + 1/(1+2|c_-|^2) \exp(-E_{2-}) \\
    P_3 &= \exp(h) + \exp(-h) \\
    P_4 &= 2|b_+|^2/(1+2|b_+|^2) \exp(-E_{1+}) + \\
        &\quad + 2|b_-|^2/(1+2|b_-|^2) \exp(-E_{1-}) + \\
        &\quad + 2|c_+|^2/(1+2|c_+|^2) \exp(-E_{2+}) + \\
        &\quad + 2|c_-|^2/(1+2|c_-|^2) \exp(-E_{2-})
\end{align*}
\]

\[
d = (K_{xy} - iD')/\sqrt{K_{xy}^2 - D'^2}
\]
Solving Eqs. (2-20) and (2-21), we find the parameters of the renormalized Hamiltonian:

\[ A_1 = \frac{(\ln P_1 + \ln P_2 + \ln P_3 + \ln P_4)}{4} \]
\[ h' = \frac{(\ln P_1 + \ln P_2)}{2} \]
\[ K_z' = \frac{(\ln P_1 + \ln P_2 - \ln P_3 - \ln P_4)}{4} \]
\[ K_{xy}' = \frac{B(K_{xy}^2 - D^2)}{(K_{xy}^2 + D^2)} \]
\[ D' = \frac{2BK_{xy}D}{(K_{xy}^2 + D^2)} \]

where

\[ B = \frac{(\ln P_4 - \ln P_3)}{4} \]

Once we have done the decimation, we can calculate the free energy per site of the system \((\ln Q)/N\) from these renormalization transformations by using the well-known formula [25]:

\[ (1/N) \ln Q_N \approx A_1/2 + (1/2)(2/N)\ln Q_N/2 \]

or,

\[ (1/N) \ln Q_N \approx (1/2) \sum_{m=0}^{\infty} \left( \frac{1}{2^m} \right) A_1(R^m(K, D, h)) \]  

(2-22)

We can obtain thereby the specific heat

\[ C/(Nk_B) = (K^2 \frac{\partial^2}{\partial K^2} + 2K_h \frac{\partial^2}{\partial K \partial h} + h^2 \frac{\partial^2}{\partial h^2})(\ln Q)/N \]  

(2-23)
the magnetization

\[ M = \partial / \partial h \left( \ln Q \right) / N \]  \hspace{1cm} (2-24)

and the susceptibility

\[ k_B T = \partial^2 / \partial h^2 \left( \ln Q \right) / N \]  \hspace{1cm} (2-25)

According to Betts's mapping relation, static thermal properties of a spin chain with parameters \{ \( K_z, K_{xy}, D, h_z \) \} are equivalent to those of a chain with parameters \{ \( K_z', K_{xy}' = \sqrt{K_{xy}^2 + D^2}, D'=0, h_z \) \}. We have used quantum decimation to calculate the specific heat for the spin chains with antisymmetric exchange, and found that the results confirm this mapping relation.

In the XY-case, a chain with \{ \( K_z=0, K_{xy}, D/K_{xy}=1, h_z=0 \) \} is equivalent to a chain with \{ \( K_z=0, K_{xy}'=\sqrt{2} K_{xy}, D'=0, h_z=0 \) \}. Since \( k_B T/K_{xy}' = (1/\sqrt{2}) k_B T/K_{xy} \). Therefore the thermodynamic properties as a function of temperature for the \( D=K_{xy} \) and \( D'=0 \) case will have different units on temperature axis. In Fig. 3 we can see that the specific heat curve of \( D/K_{xy}=1 \) is scaled by a factor of \( \sqrt{2} \) from that with \( D' \sim 0.05 \). The Katsura's exact result for symmetric exchange alone is shown in the same figure. Compared to the exact line, the \( L=2 \) line has too high a maximum. This is the same situation as that Takano and Suzuki have got [41].
Fig. 4 shows that the specific heat for isotropic ferromagnetic chains with different antisymmetric exchange has the same character as that of different XY-like anisotropic chains without antisymmetric exchange (cf. Fig. 12).
Fig. 3. Temperature dependence of the specific heat of the 1-D XY model with antisymmetric exchange. Solid curves are the present results and dashed curve is the result of Katsura [14] for the case of symmetric exchange alone.
Fig. 4. Temperature dependence of the specific heat of 1-D isotropic Heisenberg model, for various values of the antisymmetric exchange.
2.2.2 Alternating Antiferromagnetic Spin Chains

The one-dimensional magnetic chain with alternating antiferromagnetic interactions has attracted much recent attention, stimulated largely by experimental work on materials such as copper nitrate Cu(NO₃)₂·2.5H₂O [23, 49, 50] and on systems undergoing spin-Peierls transitions [4].

Theoretical treatments have focused on a model described by a reduced Hamiltonian of the form

\[ \mathcal{H} = \sum_i \left( -K_1 \sigma_i \cdot \sigma_{i+1} - K_2 \sigma_i \cdot \sigma_{i+1} - h(\sigma_i \cdot \mathbf{z}) \right) \]  

(2-26)

As described above the chain consists of spins-1/2 linked by isotropic antiferromagnetic \((K_1, K_2 < 0)\) exchange interactions which alternate in size.

For copper nitrate, Ajiro et al., Diederix et al. [23], and Bonner et al. [49] have found \(\alpha = K_2/K_1 = 0.27\), and \(K_1 T = -1.29 K\) [49, 53]. The thermodynamic properties of this material have been found to be rich in structure at low temperature and in a magnetic field. For example, the low-temperature susceptibility as a function of field (shown schematically in Fig. 5) is characterized by twin peaks at field \(H_{c1}\) and \(H_{c2}\), which arise from an excitation energy gap between a nondegenerate singlet ground state and a continuum of excited triplet states. Increasing the magnetic field depresses the Fermi level, which for \(H < H_{c1}\) and \(H > H_{c2}\) lies within the gap, and for \(H_{c1} < H < H_{c2}\) is within
Fig. 5. Susceptibility versus field at constant temperature for copper nitrate, showing peak structure near critical fields $H_{c1}$ and $H_{c2}$ (from Ref.[23]).
the band. The maxima in the density of states at the top and bottom of the band then give rise to the double-peaked response. With increasing temperature the peaks diminish in size and merge to form a single broad maximum [50].

No exact analytic approach is presently available for the Heisenberg alternating chain — in particular it has not yet proved possible to find a suitable technique based on the well-known Bethe Ansatz. Therefore the most recent theoretical treatments are approximate. The zero-field, finite-temperature properties of the alternating antiferromagnet have been investigated by Duffy and Barr [51], by Bonner et al. [52], and by Diederix et al. [23] using extrapolation of exact numerical results for rings of up to 12 spins. The field dependence of the thermodynamic properties, and the susceptibility and specific heat as functions of temperature have been calculated by Mohan and Bonner using a method due to Bulaevski based on a Hartree–Fock approximation [50].

Our purpose is to calculate static thermodynamic properties, particularly the magnetic susceptibility, in the presence of a magnetic field using the quantum decimation method. Its main advantages for this problem are that it is exact in the dimer limit (as noted above), its accuracy improves as the field strength increases, and it is rapid and versatile, allowing us to vary $H$, $T$ and $a$.
over a wider range. In order to improve this approximation, we use a sequence of scale factors \((L = 3, 5\) and \(7\)) with free boundary conditions on the cluster, and also use a large cluster \((N=6)\) with periodic boundary conditions.

Decimation for \(L = 3, 5\) and \(7\) Free-End Cluster

The basic steps of the quantum decimation method for scale factor \(L\) are first, to solve for the eigenstates and eigenvalues of the Hamiltonian of an \((L+1)\)-spin free-end cluster, and for the two-spin renormalized Hamiltonian, and then to carry out the exact decimation within one cluster. We next describe this procedure in detail for the case of alternating interactions.

In order to keep the antiferromagnetic character in the decimation procedure, (even this may not necessary for the calculating thermodynamic properties, although it is necessary to study the critical behavior), we must have an even number of spins in each cluster. Therefore the scale factor must be \(3, 5\) or \(7\), etc., and we must solve for the eigenstates and eigenvalues of \(4\), \(6\) and \(8\)-spin clusters. It is noted that even if we consider mainly isotropic initial interactions, it will be necessary from an RG viewpoint to allow for anisotropic interactions. Thus we may also treat easy-axis and easy-plane systems.

For the alternating spin chain each cluster Hamiltonian
includes 1 interaction pairs, and is either of the form 1-2-1-2 or 2-1-2-1, as illustrated in Fig. 6. $H_{b1}$ and $H_{b2}$ may then written as

$H_{b1} = \sum_{i=0}^{(L-1)/2} \left\{ -K_{1z}\sigma_{2i}\sigma_{2i+1} z - \frac{K_{1xy}}{2}(\sigma_{2i+1}^+\sigma_{2i+1}^-+\sigma_{2i}^-\sigma_{2i}^+) \right\} + \sum_{i=1}^{(L-1)/2} \left\{ -K_{2z}\sigma_{2i-1}\sigma_{2i} z - \frac{K_{2xy}}{2}(\sigma_{2i-1}^+\sigma_{2i}^-+\sigma_{2i-1}^-\sigma_{2i}^+) \right\} - \sum_{i=1}^{L-1} h_1\sigma_i z - h_1(\sigma_0 z+\sigma_L z)$

(2-27a)
\[ H_{b2} = \sum_{i=0}^{(L-1)/2} \left( -K_{2z} \sigma_{2i}^z \sigma_{2i+1}^z \right) - \frac{K_{2xy}}{2} \left( \sigma_{2i}^+ \sigma_{2i+1}^- + \sigma_{2i}^- \sigma_{2i+1}^+ \right) \] + \[ \sum_{i=1}^{(L-1)/2} \left( -K_{1z} \sigma_{2i-1}^z \sigma_{2i}^z \right) - \frac{K_{1xy}}{2} \left( \sigma_{2i-1}^+ \sigma_{2i}^- + \sigma_{2i}^- \sigma_{2i-1}^+ \right) \] - \sum_{i=1}^{L-1} h \sigma_i^z - h_2 (\sigma_0^z + \sigma_L^z) \] (2-27b)

Here
\[ h_1 + h_2 = h \] (2-28)

and
\[ \frac{h_2}{h_1} = \frac{K_2}{K_1} = \alpha \quad (K_z, K_{xy} = \beta J_z, \beta J_{xy}) \] (2-29)

We have found that the above division of the field terms for spins at the ends of each cluster preserves the symmetry of \( H_{b1} \) and \( H_{b2} \) under the interchange of indices 1 and 2, and yields the exact results in the dimer limit.

We next need solve just \( H_{b1} \). The eigenstates and eigenvalues of \( H_{b1} \) for \( L = 3, 5 \) and 7 are found by diagonalizing the exact Hamiltonian matrix, written in a suitable representation. The procedure follows closely that used by Griffiths [19], Bonner and Fisher [18], and Blöte [21] for the uniform chain, and Duffy and Barr [51] and Bonner and Blöte [52] for the alternating chain. The chain is a free-end cluster. Since \( H_{b1} \) and the \( Z \) component of
total spin operator

\[
\sigma_z = \sum_{i=0}^{L} \sigma_i^z
\]  \hspace{1cm} (2-30)

commute, a convenient choice of basis function \( |P_z⟩ \) are again the eigenfunctions of \( \sigma_z \) which are direct products of the eigenfunctions of \( \sigma_i^z \). This yields \( H_{b1} \) as a

\[
2(L+1) \times 2(L+1)
\]

matrix in block form in which the largest block is

\[
\begin{pmatrix}
(L+1) \\
(L+1)/2
\end{pmatrix}
\times
\begin{pmatrix}
(L+1) \\
(L+1)/2
\end{pmatrix}
\]

and each block corresponds to a single \( \sigma_z \).

A further reduction of block size can be obtained by introducing a mirror reflection operator \( R \) \([21,52]\), which interchanges the spin vectors at sites \( i \) and \( L-i \). \( R \) commutes with \( H_{b1} \). We can use \( R \) to introduce the simple symmetric basis states

\[
|P_+ Z⟩ = |P_z⟩ + R|P_z⟩
\]

and antisymmetric states

\[
|P_- Z⟩ = |P_z⟩ - R|P_z⟩
\]

For \( L=3,5 \) and \( 7 \), we list all block sizes for \( H_{b1} \) in Table 4.

We find the eigenfunctions

\[
|m⟩ = \sum_i a_i(m)|i⟩
\]

and eigenvalues \( E_m \) numerically for the \((L+1)\)-spin cluster.
Table 4. The block sizes for $H_{b1}$ of $L = 3$, 5 and 7. Since the block size for $\sigma z \langle 0 \rangle$ is the same as that of $\sigma z \rangle 0$, we just list that of $\sigma z \rangle 0$.

$L = 3$

$\sigma z \quad 4 \quad 2 \quad 0$

| $|P_+\rangle$ | $|P_+4\rangle$ | $|P_+2\rangle$ | $|P_-2\rangle$ | $|P_+0\rangle$ | $|P_-0\rangle$ |
|----------------|----------------|----------------|----------------|----------------|----------------|
| Dim.           | 1              | 2              | 2              | 4              | 2              |

$L = 5$

$\sigma z \quad 6 \quad 4 \quad 2 \quad 0$

| $|P_+\rangle$ | $|P_+6\rangle$ | $|P_+4\rangle$ | $|P_-4\rangle$ | $|P_+2\rangle$ | $|P_-2\rangle$ | $|P_+0\rangle$ | $|P_-0\rangle$ |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Dim.           | 1              | 3              | 3              | 9              | 6              | 10             | 10             |

$L = 7$

$\sigma z \quad 8 \quad 6 \quad 4 \quad 2 \quad 0$

| $|P_+\rangle$ | $|P_+8\rangle$ | $|P_+6\rangle$ | $|P_-6\rangle$ | $|P_+4\rangle$ | $|P_-4\rangle$ | $|P_+2\rangle$ | $|P_-2\rangle$ | $|P_+0\rangle$ | $|P_-0\rangle$ |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Dim.           | 1              | 4              | 4              | 16             | 12             | 28             | 28             | 38             | 32             |

Table 5. The four eigenstates and eigenvalues of a two spin cluster.

| $|n\rangle$ | $E_n$ |
|----------------|----------------|
| $|1\rangle$ | $|\uparrow\uparrow\rangle$ | $E_1' = -K_{1z}' - 2h_1'$ |
| $|2\rangle$ | $|\downarrow\downarrow\rangle$ | $E_2' = -K_{1z}' + 2h_1'$ |
| $|3\rangle$ | $1/2 \left| \uparrow\downarrow + \downarrow\uparrow \right>$ | $E_3' = K_{1z}' - 2K_{1xy}'$ |
| $|4\rangle$ | $1/2 \left| \uparrow\downarrow - \downarrow\uparrow \right>$ | $E_4' = K_{1z}' + 2K_{1xy}'$ |
The renormalized Hamiltonian $H_{b1}'$ has eigenstates $|n\rangle$ and eigenvalues $E_n'$ which we shown in Table 5.

Next we decimate within one cluster

$$\exp\{ A_1-H_{b1}' \} = \text{Tr}' \exp\{ -H_{b1} \} = \text{Tr}' \sum_{m} |m><m| \exp\{-E_m\}$$

$$= \text{Tr}' \sum_{m} \left( \sum_{i} a_i(m)|i\rangle \right) \left( \sum_{j} a_j(m)|j\rangle \right) \exp\{-E_m\}$$  \hspace{0.5cm} (2.31)

Here $\text{Tr}'$ means to take the partial trace over all $(L-1)$ intermediate spins. Here we list the all situations that will be encountered:

$$\text{Tr}' a^2 |\uparrow A\uparrow\rangle<\uparrow A\uparrow| = a^2 |1\rangle<1|$$

$$\text{Tr}' a^2 |\downarrow A\downarrow\rangle<\downarrow A\downarrow| = a^2 |2\rangle<2|$$

$$\text{Tr}' a^2/2 |\uparrow A\uparrow\downarrow\uparrow A\uparrow\rangle<\uparrow A\uparrow\downarrow\uparrow A\uparrow| = a^2 |3\rangle<3|$$

$$\text{Tr}' a^2/2 |\uparrow A\uparrow\downarrow\downarrow A\uparrow\rangle<\uparrow A\uparrow\downarrow\downarrow A\uparrow| = a^2 |4\rangle<4|$$

$$\text{Tr}' 1/2 \left( a |\uparrow A\uparrow\downarrow B\uparrow\rangle+b |\uparrow B\uparrow\downarrow A\uparrow\rangle \right) \left( a<\uparrow A\uparrow\downarrow B\uparrow|+b<\uparrow B\uparrow\downarrow A\uparrow| \right) =$$

$$= (a+b)^2 |3\rangle<3| + (a-b)^2 |4\rangle<4|$$

$$\text{Tr}' 1/2 \left( a |\uparrow A\uparrow\downarrow B\uparrow\rangle+b |\uparrow B\uparrow\downarrow A\uparrow\rangle \right) \left( a<\uparrow A\uparrow\downarrow B\uparrow|+b<\uparrow B\uparrow\downarrow A\uparrow| \right) =$$

$$= (a-b)^2 |3\rangle<3| + (a+b)^2 |4\rangle<4|$$

$A$ and $B$ are the configurations of the $(L-1)$ intermediate spins. We thereby find

$$\sum_{n=1}^{4} |n\rangle<n| \exp\{A_1-E_{n}'\} = \sum_{n=1}^{4} |n\rangle<n| \mathbb{P}_n$$
By solving these equations, the parameters for the renormalized Hamiltonian $H_{b1}'$ are found to be as follows:

$$\begin{align*}
A_1 &= \left( \ln P_1 + \ln P_2 + \ln P_3 + \ln P_4 \right) / 4 \\
K_{1z}' &= \left( \ln P_1 + \ln P_2 - \ln P_3 - \ln P_4 \right) / 4 \\
K_{1xy}' &= \left( \ln P_3 - \ln P_4 \right) / 4 \\
h_1' &= \left( \ln P_1 - \ln P_2 \right) / 4
\end{align*}$$

Permuting indices 1 and 2, we find the parameters $A_2$, $K_{2z}'$, $K_{2xy}'$, and $h_2'$ for the renormalized cluster Hamiltonian $H_{b2}'$. The renormalized field is thus given by

$$h' = h_1' + h_2'.$$

The free energy is calculated by iteration:

$$\left( \ln Q \right)/N \cong 1/(2L) \sum_{m=0}^{1/(Lm)} (A_1 + A_2) (R(m)[K,\alpha,h])$$

(2-32)

We may check the procedure in the dimer and Ising cases, for which the decimation method is exact. The free energy for the isotropically interacting dimers is

$$\left( \ln Q \right)/N = 1/2 \ln \left\{ \exp(K+2h) + \exp(K-2h) + \exp(K) + \exp(-3K) \right\}$$

While for the Ising case

$$\left( \ln Q \right)/N = \ln \left\{ \exp(K) \cosh h + \sqrt{\exp(2K) \sinh^2 h + \exp(-2K)} \right\}$$
From the free energy, one can calculate specific heat, magnetization and susceptibility using formulas (2-23, 24 and 25) and numerical differentiation.

Note that in Eq.2-31 every iteration needs two decimations of the alternating chain. Since we intend to calculate thermal properties, and do not expect any singularities in the free energy (i.e. phase transitions with the appearance of an order parameter) there remains considerable freedom in the choice of rescaling steps. An alternative method is shown in Fig. 7. In this iteration scheme, after one decimation one retains an alternating spin chain and can continue as before. In this way, every iteration needs just one decimation, reducing computation time. Using this iteration procedure, the formula for the free energy becomes

\[
\frac{(\ln Q)}{N} \approx \frac{1}{(L+1)} \sum_{m=0} 1/[(L+1)/2]2 A_1(R(m)\{K,\alpha, h\})
\]

(2-33)

\(L\) is still the scale factor, 3, 5 or 7. The results using this alternative method will be discussed below.
Fig. 7. **Alternative iteration method for free energy calculation.**

**Periodic Boundary Conditions: the 6-Spin Ring**

An alternative to using a larger scale factor is to keep the scale factor constant but increase the number of spins treated at once. This approach also reduces the errors which occur due to noncommuting operators. However, a cluster with free boundary conditions will produce renormalized interactions which are not uniform, but vary with their position in the cluster. Periodic boundary conditions eliminate this problem, and have been found for example to be important in obtaining reliable RG results on two dimensional classical (Ising) systems. The renormalization process for a ring is also aided by the N/2-fold translational symmetry (for alternating interactions), by which the diagonalization of the
Hamiltonian is simplified. (This reduction in computer time applies also to the finite chain extrapolations of Bonner and others, which customarily employ rings.)

For alternating interactions, a 6-spin ring is the smallest possible cluster which can be decimated. Renormalizing (see Fig. 8b,c) to 3 spins yields uniform rather than alternating interactions, but for the purpose of calculating the free energy this is nonetheless reasonable, and we have in fact found that it gives reliable results.

We next briefly discuss the technical problems which arise in renormalizing a ring of spins. The general decimation formula is

\[ \exp\{ A_1 - H_b' \} = \text{Tr}' \exp\{-H_b\} \quad (2-34) \]

For the free-end cluster decimations, the decimated Hamiltonian \( H_{b'} \) has four eigenstates \( |n\rangle \) and eigenvalues \( E_{n'} \). After decimation we find

\[
\sum_{n=1}^{4} |n\rangle\langle n| \exp\{ A_1 - E_{n'} \} = \sum_{n=1}^{4} |n\rangle\langle n| P_n
\]

This yields four equations in four unknowns—the constant \( A_1 \) and three parameters of the renormalized Hamiltonian \( H_{b'}: K'_z, K_{xy}', \text{ and } h' \).
Fig. 8. Bond-moving and spin ring decimation.
(a) The ensemble of six-spin rings arises from infinite spin chain by bond-moving approximation.
(b,c) The spin ring before and after decimation. Note that the six-spin alternating ring transforms into three-spin uniform ring.
(d) The ensemble of spin ring reverts to spin chain by bond-moving approximation.
For the three spin ring,

\[
H_b' = -K_z'(12) + (23) + (13) - K_{xy'}((12)_A + (23)_A + (13)_A)
- h'((1) + (2) + (3))
\]  

(2-35a)

For simplicity we have introduced the symbols

\[
(ij) = \sigma_i^z \sigma_j^z \\
(ij)_x = \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \\
(i) = \sigma_i^z
\]  

(2-36)

Using translation symmetry, one finds the eight eigenstates \( |n\rangle \), and eigenvalues \( E_n' \), which are listed in the Table 6a. We see that there are two doublets, characterized by momenta \( k_1 \) and \( k_2 \), which are linear combinations of product states with complex coefficients. One can use the mirror reflection operator \( R \) (see p.35) to make the expansion coefficients real. The results of this procedure are shown in Table 6b.

The six different eigenvalues in general determine six unknowns in the decimation procedure, and therefore two additional interaction terms in \( H_b' \), Eq.(2-35a). It is of course normal that the RG produces new interaction terms, and as a first order approximation, these typically are truncated at each step. If we want to keep just the symmetric bilinear interaction and the longitudinal field terms in the Hamiltonian, the only interactions which we
can add on the uniform 3-spin ring are 3-spin terms. Thus we add two three-spin interaction terms to $H_b'$:

$$
H_b' = -K_Z'((12)+(23)+(13)) - K_{xy}'((12)_{\perp} + (23)_{\perp} + (13)_{\perp}) - h'((1)+(2)+(3)) + T(123) + S((12)_{\perp}(3) + (23)_{\perp}(1) + (13)_{\perp}(2))
$$

(2-35b)

Here we use the same symbols as those of Eq. (2-36)

$$(ijk) = \sigma_i^z \sigma_j^z \sigma_k^z$$

$$(ij)_{\perp}(k) = (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \sigma_k^z$$

The new eigenstates are the same as those of Eq. (2-35a) the new eigenvalues are listed in Table 6b.

For the 6-spin alternating ring

$$
H_b = -K_Z((12)+(34)+(56)+a[(23)+(45)+(16)]) - K_{xy}((12)_{\perp} + (34)_{\perp} + (56)_{\perp} + a[(23)_{\perp} + (45)_{\perp} + (16)_{\perp}]) - h((1)+(2)+(3)+(4)+(5)+(6))
$$

The original Hamiltonian matrix is thus 64x64, but can be block-diagonalized by considering rotational, translational and mirror symmetries. Choosing eigenstates of $\sigma^z$ gives a largest block which is 20x20. Further use of the operators $T$ (translation) and $R$ reduces the largest submatrix to 5x5 with all entries real (see Table 7). This is then rapidly diagonalized numerically.
Table 6. Eigenstates and eigenvalues of 3-spin ring Hamiltonian $H'$: (a) complex eigenvectors for Eq. (2-35a), (b) real eigenvectors for Eq. (2-35a) and (2-35b).

(a)

| $|n\rangle$ | $E_n'$ |
|---|---|
| $|\uparrow\uparrow\uparrow\rangle$ | $-3K_z'-3h'$ |
| $|\downarrow\downarrow\downarrow\rangle$ | $-3K_z'+3h'$ |
| $|\uparrow k_j\rangle$ | $K_z'-h'-4K_{xy}'\cos k_j$ |
| $|\downarrow k_j\rangle$ | $K_z'+h'-4K_{xy}'\cos k_j$ |

$^c$: $|\uparrow k_j\rangle = \frac{1}{\sqrt{3}} |\uparrow\uparrow\uparrow+e_j1\uparrow\downarrow+e_j2\uparrow\uparrow\uparrow\rangle$

$|\downarrow k_j\rangle = \frac{1}{\sqrt{3}} |\downarrow\downarrow\downarrow+e_j1\downarrow\uparrow+e_j2\downarrow\uparrow\uparrow\rangle$

( $e_j1 = \exp(ik_j)$, $e_j2 = \exp(i2k_j)$, $k_j = 2\pi j/3$, and $j = 0, 1$ and $2$.)

(b)

| $|n\rangle$ | $E_n'^{\circ}$ | $E_n'^{\circ\circ}$ |
|---|---|---|
| $|1\rangle=|\uparrow\uparrow\uparrow\rangle$ | $-3K_z'-3h'$ | $-3K_z'+T-3h'$ |
| $|2\rangle=|\downarrow\downarrow\downarrow\rangle$ | $-3K_z'+3h'$ | $-3K_z'-T+3h'$ |
| $|3\rangle=1/\sqrt{3} |\uparrow\uparrow\uparrow+\uparrow\downarrow+\uparrow\uparrow\uparrow\rangle$ | $K_z'-4K_{xy}'-h'$ | $K_z'-4K_{xy}'-T+4S-h'$ |
| $|4\rangle=1/\sqrt{6} |\downarrow\downarrow\downarrow-\downarrow\uparrow-\downarrow\downarrow\downarrow\rangle$ | $K_z'+2K_{xy}'-h'$ | $K_z'+2K_{xy}'-T-2S-h'$ |
| $|5\rangle=1/\sqrt{2} |\uparrow\downarrow+\uparrow\uparrow\uparrow\rangle$ | $\cdot\cdot\cdot$ | $\cdot\cdot\cdot$ |
| $|6\rangle=1/\sqrt{3} |\uparrow\uparrow\uparrow+\uparrow\downarrow+\uparrow\uparrow\uparrow\rangle$ | $K_z'-4K_{xy}'+h'$ | $K_z'-4K_{xy}'+T-4S+h'$ |
| $|7\rangle=1/\sqrt{6} |2\downarrow\downarrow\downarrow-\downarrow\uparrow-\downarrow\downarrow\downarrow\rangle$ | $K_z'+2K_{xy}'+h'$ | $K_z'+2K_{xy}'+T+2S+h'$ |
| $|8\rangle=1/\sqrt{2} |\uparrow\uparrow\uparrow-\uparrow\downarrow\uparrow\uparrow\rangle$ | $\cdot\cdot\cdot$ | $\cdot\cdot\cdot$ |

$^c$: $E_n'^{\circ}$ is for Eq. (2-35a) and $E_n'^{\circ\circ}$ is for Eq. (2-35b) (including 3-spin interactions).
Table 7. The dimensions of block matrices of 6-spin alternating ring Hamiltonian. Here we just list those for non-negative Z component of total spin.

<table>
<thead>
<tr>
<th>σ^Z</th>
<th>6</th>
<th>4</th>
<th>2</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>by σ^Z</td>
<td>1</td>
<td>6</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>by T,R</td>
<td>1,1,1,1,1,1</td>
<td>1,4,5,5</td>
<td>4,4,3,3,3,3</td>
<td></td>
</tr>
</tbody>
</table>

Decimation procedure. Substituting the eigenstates and eigenvalues of both three spin and six spin ring Hamiltonians into Eq(2-31), we get

\[ A_1 = \sum_{n=1}^{8} \sum_{m=1}^{64} E_{n'} |n><n| = \ln \text{Tr}' \sum_{m=1}^{64} \exp(-E_{m'}) |m><m| \]

(2-37)

In the decimation procedure, there are the following situations that need to be treated:

For \( \sigma^Z = 3 \) in the decimated (3-spin) ring,

\[ \text{Tr}' \exp(-E_{m'}) |↑A↑B↑C><↑A↑B↑C| = \exp(-E_{m'}) |1><1| \]

where \( |ABC\rangle \) is any state function of the decimated spins.

For \( \sigma^Z = 1 \),

\[ I_{1^+} = \text{Tr}' \exp(-E_{m'}) |a_1↑A↑B↑C+a_2↑A↑B↑C+a_3↑A↑B↑C><a_1↑A↑B↑C+a_2↑A↑B↑C+a_3↑A↑B↑C| \]

\[ = \exp(-E_{m'}) |a_1↑↑↑+a_2↑↑↑+a_3↑↑↓><a_1↑↑↑+a_2↑↑↑+a_3↑↑↓| \]

We can expand this state using basis states: \( |3\rangle \), \( |4\rangle \) and \( |5\rangle \) in Table 6b:
\[ |a_1 \uparrow \uparrow + a_2 \uparrow \uparrow + a_3 \uparrow \uparrow \rangle = b_3 |3 \rangle + b_4 |4 \rangle + b_5 |5 \rangle \]

and find

\[
\begin{vmatrix}
 b_3^2 & b_3 b_4 & b_3 b_5 \\
 b_3 b_4 & b_4^2 & b_4 b_5 \\
 b_3 b_5 & b_4 b_5 & b_5^2 \\
\end{vmatrix}
\]

The same situations obtain for \( \sigma z = -3 \) and \(-1 \). As a result, we find from Eq.(2-37)

\[ A_1 - H_b' = \ln B \]

Here \( B \) is a symmetric block-diagonalized matrix that has the form

\[
B = \begin{bmatrix}
1x1 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 3x3
\end{bmatrix}
\]

We can easily take the logarithm of the matrix \( B \),

\[ \log B = U ( \log U^{-1} B U ) U^{-1} \]

where \( U \) is an orthogonal matrix that diagonalizes \( B \):

\[ B' = U^{-1} B U \]

We find finally that
The left side of this equation is diagonal. If the right side is not, we should have included more interaction terms in the original Hamiltonian. Fortunately, we have examined the more general situation— the alternating, anisotropic spin chain in large field, $\alpha < 1$, $K_z = K_{xy}$, and $h > 0$, and find that the right side of Eq. (2-39) is always diagonal. In fact,

$$U (\log U^{-1} B U) U^{-1} = \sum_{n=1}^{8} |n><n| P_n$$

where $P_4 = P_5$ and $P_7 = P_8$, corresponding to $E_4' = E_5'$ and $E_7' = E_8'$. Therefore the Hamiltonian of the decimated 6-spin ring is consistent with that of a 3-spin ring with a constant term and five interactions.

As a consequence we find:

$$
\begin{align*}
A_1 - 3K_z' + T & \quad \quad -3h' = P_1 \\
A_1 - 3K_z' - T & \quad \quad +3h' = P_2 \\
A_1 + K_z' - T + 4S - 4K_{xy}' - h' & = P_3 \\
A_1 + K_z' - T - 2S + 2K_{xy}' - h' & = P_4 \\
A_1 + K_z' + T - 4S - 4K_{xy}' + h' & = P_6 \\
A_1 + K_z' + T + 2S + 2K_{xy}' + h' & = P_7 
\end{align*}
$$

(2-40)
Solving this set of equations gives the constant $A_1$ and the parameters of the renormalized Hamiltonian $H_{b'}$, i.e. $K_{z'}, T, S, K_{xy'}$ and $h'$.

In summary, this approximate decimation RG has the following characteristics:

1. It changes the antiferromagnetic chain into a ferromagnetic one, since this decimation is for scale factor $L=2$.

2. The renormalized 3-spin interaction terms, $T$ and $S$ (see Eq. (2-35b)) are always smaller by more than one order of magnitude than the one and two spin interaction terms, and grow slowly with field. It is therefore reasonable to truncate the 3-spin terms.

From the viewpoint of bond-moving approximation [54], a 6-spin ring can be considered to come from an infinite spin chain after moving bonds. When we complete one decimation, we get an ensemble of isolated 3-spin rings. We can turn it back into a spin chain by applying the bond-moving procedure a second time (see Fig. 8). By repeating procedure one again develops the free energy formula

$$\frac{(\ln Q) / N}{(1/6) \sum_{m=0}^{(1/(2m)) A_1(R(m), K, a, h)}}$$
Thermodynamic Properties

We have introduced above the approximate decimation procedure for \( L = 3, 5 \) and 7 free-end spin clusters and for the \( N = 6 \) ring. The results of the specific heat and susceptibility calculations in a variety of cases are shown in Fig. 9 through 22, where appropriate they are compared with the finite-chain extrapolations of Ref.[18,57].

In Fig. 9 are plotted the ferromagnetic specific heats for uniform isotropic Heisenberg coupling in zero field. The results of \( L = 3, 5 \) and 7 free-end cluster decimation are successively closer to the Bonner-Fisher estimates, with respective deviations at \( k_B T/J = 1.0 \) of 8.2\%, 5.1\% and 3.6\%. The low-temperature results are not quantitatively accurate, but the successive approximations appear to be converging to an important feature of the 1-D ferromagnet, namely a specific heat falling to zero as \( T \rightarrow 0 \). In the temperature region \( k_B T/J > 1.0 \) the ring calculation gives better results than those by \( L=7 \) open chain decimation, but this is not the case at the lower temperatures.

The same comparison, for isotropic antiferromagnetic coupling, is shown in Fig. 10. At \( k_B T/J = 1.0 \) the deviation from the finite chain extrapolations is in every case larger than for ferromagnetic exchange. At the higher temperature region \( (k_B T>1.0) \) the ring calculation again yields the best agreement. At low-temperatures there is
apparent convergence of the free-end cluster results to a
linear behavior of C(T). (The antiferromagnetic energy
spectrum is proportional to momentum k for small k, as
opposed to k² in the ferromagnetic case.) Approximations
involving finite numbers of spins, of course, will always
show exponential behavior of C(T) for sufficiently low
temperature.

Fig. 11 shows the specific heat for different
anisotropy factors γ = J_{xy}/J_z = 1.0, 0.5 and 0 in the case
of easy-axis (Ising-like) Heisenberg ferromagnetic and
antiferromagnetic chains. A single RG technique has been
used, namely the L = 5 free-end cluster method. The thermal
behavior of the pure Ising chain is of course the same for
either ferromagnetic and antiferromagnetic interactions. It
is known that there exists an energy gap to the first
excited state for all γ<1 [17,55,56], which vanishes as 1−γ
in the ferromagnetic case and with an essential singularity
( ~ exp(-cst./√1−γ ) ) for antiferromagnetic couplings.
Our approach, however, is not sufficiently sensitive at low
T to show evidence of these effects.

Fig. 12 displays the specific heats for easy-plane
(XY-like) chains with γ = 1, 2 and ∞. Again the L = 5 free-
end cluster approach has been used, and we remark that pure
XY chains have the same specific heat for either sign of
the coupling. There is no energy gap for either the ferro-
or the antiferromagnetic case, so that \( C \) should approach zero in power law fashion. Here too, however, the RG gives no clear indication of the detailed low-\( T \) behavior.

The susceptibility results are in general more accurate than those for specific heat obtained by the same methods. For instance, for the Heisenberg chain with ferromagnetic coupling (see Fig. 13), the zero field susceptibility RG results (\( L=3 \) open chain) at \( k_B T/J = 1.0 \) differ from the finite chain (\( N=8 \) ring) predictions by \( \sim 3\% \), and those for the specific heat, by \( \sim 8\% \) (see Fig. 9). The same trend is apparent in the isotropic Heisenberg antiferromagnetic case, as may be seen by comparing Fig. 10 and Fig. 14. The same situation occurs in the finite chain calculations, where the susceptibilities are surprisingly close to those of the infinite system [14].

We also find that the results of the decimation RG for thermodynamic properties in nonzero field are more accurate than those in zero field. This situation is also similar to that in the finite chain extrapolations, where the convergence with \( N \) is appreciably more rapid in a field than for \( H=0 \) [18]. Susceptibility versus temperature curves for the ferromagnetic Heisenberg chain for several values of applied field are displayed in Fig. 13. We find that they are in close agreement with the results for 8-spin finite ring [18], also shown.
The susceptibility versus temperature at constant field for the uniform antiferromagnetic chain is shown in Fig. 15. At the critical field value $H/J = 4$ (for which the zero-temperature magnetization saturates) the calculated $\chi$ appears to diverge as $T \to 0$, while for larger field it approaches zero, both in accordance with the known behavior [18]. For small fields, $\chi$ should approach a finite zero-temperature limit, but the RG results do not generally allow for reliable extrapolation in these cases. The detailed view of the $H=0$ situation provided in Fig. 14 indicates the correct trend with increasing $L$.

The specific heat vs. temperature curves at constant magnetic field for the antiferromagnet are shown in Fig. 16. Exact finite-chain results of Ref.[18] for $H/J = 0$ and 5 are included for comparison. (The displayed curves are the means of 9- and 10-spin chain calculations.) The improved agreement in the high-field case is easily seen. For $H$ greater than the critical field little difference can be noted between the two methods, although for $H<4$ the agreement is poorer. In particular the pronounced shoulder at $T = 0.3$ and $H = 3$ is thought to be spurious.

The improvement of the results for susceptibility over those for specific heat, and of the finite-field results over those in zero field, appear to be related to the fact that in finite field the couplings -- both
transverse and longitudinal — renormalize rather more rapidly to zero than in the cases when the field is absent. On the other hand, the renormalized field always increases with each iteration for ferromagnetic chains, while for antiferromagnetic coupling it decreases at a rate that is dependent on the division of the Zeeman terms at the cluster ends. In any case, the exchange constants always decrease faster than the fields. Relatively speaking the smaller the exchange, and the larger the Zeeman term, the more accurate the RG results.

**Alternating antiferromagnetic chain**

We next turn our attention to the antiferromagnet with alternating couplings. Since the quantum decimation method is exact in the dimer limit, and the uniform chain results lead us to expect greater reliability in the case of magnetic properties, we have calculated the susceptibilities for the case $\alpha=0.27$, corresponding to copper nitrate, scanning the field at constant temperature $k_B T/J = 0.05$.

The $L=3$ open chain method gives peaks at lower and upper critical fields $H_{c1}/J_1=2.1$, and $H_{c2}/J_1=2.5$, respectively. While the latter agrees closely with result (2.54) of reference 49, the lower critical field is higher than the quoted value (1.675) by about 25% (see Fig. 17).
Increasing the block size to \( L = 5 \) and \( 7 \) gives the results shown in Fig. 18. The lower critical field falls as \( L \) increases, reaching a value at \( L = 7 \) which is only about 10\% in excess of that given by finite chain extrapolation. We can also see that as the block size increases the peak structure becomes obscure and a third (middle) peak becomes apparent, the origin of which will be discussed below.

We have also found the susceptibility by using the second iteration method (Eq.(2-33)) based on free-end clusters. Here we still use the division of the Zeeman terms for spins at the ends of each cluster given by Eq.(2-29). The results of this procedure are shown in Fig. 19. They have the same character as those of Fig. 18, but the peak structure by the second iteration method is clearer than that by the first. We are able to carry out a linear extrapolation [56] of \( H_{c1} \) vs. \( 1/L \), giving \( H_{c1} = 1.61 \) in the large-cell limit.

We have repeated the above computation with \( L=3 \) free-end clusters without dividing Zeeman terms between neighboring clusters — that is we let \( h_1 = h \) and \( h_2 = 0 \). In this approximation the lower critical field appears at about 1.8 — a slight improvement —, but no upper critical field was found out to \( H/J = 2.8 \). At slightly higher temperature, \( k_{BT}/J=0.08 \), the upper critical field appears
at about 2.7 (Fig. 20). However even at high fields the magnetization still does not saturate.

It is apparent that the treatment of the Zeeman term for the end spins has a marked effect on the results. In the last instance ($h_1 = h$, $h_2 = 0$) we have checked the iteration step by step and found that in high field ($H/J > 2.3$), at the first iteration the ground state is ferromagnetic. With successive iterations, the magnetic field decreases at the same rate as does the coupling constant, until at last the ground state is no longer ferromagnetic. Thus the magnetization is not saturated, or in other words the upper critical field is shifted to a larger value.

In Fig. 19 we considered the following division of the field terms for the end spins:

$$h = h_1 + h_2, \text{ and } h_2/h_1 = \alpha.$$  

Hence only part of field $h_1$ that applies to the end spins takes part in the iteration. Therefore in the next iteration we will leave a larger field term

$$R\text{h} = h_2 + h'.$$

Thus we can keep the ground state is ferromagnetic state during successive iterations, and the magnetization will be saturated.

To summarize, by taking $h_2/h_1 = \alpha$ (Fig. 19) we find an improved upper critical field value, while by taking
\( \frac{h_2}{h_1} = 0 \) (Fig. 20) we get a better lower critical field value.

The entire Zeeman problem for the end spins is of course absent with periodic boundary conditions. We find in fact that the 6-spin ring gives a more accurate lower critical field value. The susceptibilities for the alternating antiferromagnetic chain along several different isotherms are shown in Fig. 21. We can see that as the temperature rises the peaks diminish in size and merge to form a single broad maximum. A third middle peak again appears at low temperature, which we attribute to the use of finite blocks. We show the energy spectrum of an alternating ring of six spins as a function of the applied field in Fig. 22. Roughly speaking (since this applies to a single iteration) the first and last ground state level crossing points determine the lower and upper critical field values, while the intermediate level crossing corresponds to the middle peak. This appears only as a finite block effect, and causes difficulty for extrapolating the results to the large-ring limit. It is probable that the number of intermediate peaks would increase with the block size until, for the infinite chain, they are obscured, only leaving the two peaks that correspond to two critical fields.
Fig. 9. Variation of specific heat with temperature for ferromagnetic Heisenberg chains by decimation using $L = 3$, 5 and 7 free-end cluster (solid line), and 6-spin ring (dashed line). Comparison is made with the numerical extrapolations of Ref.[18] (dotted line).
Fig. 10. Variation of specific heat with temperature for antiferromagnetic isotropic Heisenberg chains by decimation using L=3, 5 and 7 free-end clusters (solid line), and 6-spin ring (dashed line). Comparison is made with the predictions of Bonner and Fisher [18] (dotted line).
Fig. 11. Specific heat versus temperature at constant anisotropy $\gamma$ for Ising-like spin chains ($L=5$ free-end clusters). $F$ and $AF$ denote the spin chains with ferro- and antiferromagnetic couplings.
Fig. 12. Specific heat versus temperature at constant anisotropy $\gamma$ for XY-like spin chains ($L=5$ free-end clusters).
Fig. 13. Susceptibility of isotropic spin chain with ferromagnetic coupling at constant magnetic field. Solid lines: $L=3$ decimation RG, dashed lines: exact 8-spin ring results of Ref.[18].
Fig. 14. Susceptibility of antiferromagnetic isotropic spin chain in zero magnetic field. Shown are for comparison are results by $L=3, 5$ decimation RG (solid lines), and from Ref.[18] the exact 4- and 10-spin ring calculations (dashed lines) and the estimated limiting curve by finite chain extrapolation (dotted line).
Fig. 15. Susceptibility versus temperature for antiferromagnetic isotropic spin chain at constant magnetic field.
Fig. 16. Specific heat versus temperature for antiferromagnetic isotropic spin chain at constant magnetic field. Solid lines: \( L = 5 \) decimation RG, dashed lines: 9- and 10-spin ring results for \( H/J = 5 \) and the dotted line: estimated limiting line for \( H/J = 0 \) from Ref.[18].
Fig. 17. Susceptibility of the alternating linear chain with alternating ratio $a=0.27$ as a function of field for two different temperatures. Solid lines: $L=3$ decimation RG, dashed lines: of Ref.[50].
Fig. 18. Susceptibility of the alternating linear chain with $a=0.27$, versus field at constant temperature $k_B T/J = 0.05$. L=3, 5 and 7 decimation approaches are shown, using the iteration method of Eq.(2-32).
Fig. 19. Susceptibility of the alternating chain with $\alpha=0.27$, versus field at constant temperature $k_BT/J=0.05$. $L=3, 5$ and 7 decimation approaches are shown, using the iteration method of Eq.(2-33).
Fig. 20. Susceptibility of the alternating linear chain with $a=0.27$ versus field for $k_BT/J=0.08$, $L=3$ decimation with iteration Eq. (2-33) and Zeeman terms for the end spins taken with $h_1=h$ and $h_2=0$. 
Fig. 21. Susceptibility of the alternating linear chain with $a=0.27$ versus field at constant temperature, using 6-spin ring decimation.
Fig. 22. Energy spectrum of an alternating ring of six spins as a function of the magnetic field.
2.3 DECIMATION FOR CHAINS WITH ARBITRARY FIELD DIRECTION

Since it may be difficult in an experiment to align the magnetic field exactly along a definite crystal axis, it is important to learn the effect of a transverse field on the magnetic response. Until now, quantum RG calculations and finite chain extrapolations for 1-D spin chains have been primarily concerned with the case of a longitudinal field — that is, with the field along an easy axis (Ising case) or perpendicular to an easy plane (XY case). Bonner and Fisher [18] have calculated the T=0 perpendicular susceptibility for finite chains of up to 10 spins, and Takano and Suzuki [41] have discussed the magnetic exponents for longitudinal and transverse fields using a bond-moving scheme to extend 1-D RG methods to 2- and 3-D systems. In the following section we present an extension of the decimation RG method which allows us to calculate thermodynamic properties in the presence of a field oriented in an arbitrary direction.

If there are both X and Z components of the field, the Z component of total spin, $\sigma^Z$, no longer commutes with the Hamiltonian. The calculation for larger sized clusters becomes more difficult and we therefore extend the quantum decimation RG with $L = 3$ free-end clusters to the general field case. The decimation transformation is still that of Eq. (2-34)
\[
\exp \{ A - H_b' \} = \text{Tr} \exp \{ -H_b \}
\]  

(2-34)

where \( H_b \) is the Hamiltonian of four-spin cluster and \( H_b' \) is the renormalized Hamiltonian of two-spin cluster. We again begin by solving for the eigenstates and eigenvalues of \( H_b \) and \( H_b' \).

**Two-spin cluster.** The renormalized Hamiltonian of two-spins is now

\[
H_{b'} = -K_z' \sigma_0^z \sigma_L^z + K_{xy}/2 \left( \sigma_0^+ \sigma_L^- + \sigma_0^- \sigma_L^+ \right) - h_z' \left( \sigma_0^z \sigma_L^z \right) - h_x'/2 \left( \sigma_0^+ \sigma_0^- + \sigma_L^+ \sigma_L^- \right)
\]  

(2-41a)

where Eq. (2-9) has been used. There are two problems that we must treat. First, from the viewpoint of the RG the \( h_x \) breaks the symmetry in XY-plane. As a consequence, we need to allow for anisotropic couplings in the XY-plane, even though at the beginning we have isotropic interactions. As a result we expect the renormalized Hamiltonian of two spins to be of the form:

\[
H_{b'} = -K' \sigma_0^z \sigma_L^z - D_x' \sigma_0^x \sigma_L^x - D_y' \sigma_0^y \sigma_L^y - h_z' \left( \sigma_0^z \sigma_L^z \right) - h_x'/2 \left( \sigma_0^+ \sigma_0^- + \sigma_L^+ \sigma_L^- \right)
\]  

(2-41b)
We have introduced

\[ DS = (D_x + D_y)/2 \quad \text{and} \quad DA = (D_x - D_y)/2 \quad (2-42) \]

and have used relation (2-9) to get

\[ \sigma_0^x \sigma_L^x - \sigma_0^y \sigma_L^y = (\sigma_0^+ \sigma_L^+ + \sigma_0^- \sigma_L^-)/2 \]

Second, we cannot in general solve for the four eigenstates and eigenvalues of Hamiltonian (2-41b) analytically. Instead we choose the following basis set,

\[ \begin{align*}
|1\rangle &= |+ + \rangle \\
|2\rangle &= |+ - \rangle \\
|3\rangle &= |- + \rangle \\
|4\rangle &= |- - \rangle 
\end{align*} \quad (2-43) \]

and write Hamiltonian (2-41b) as

\[ H_b'' = \begin{pmatrix}
-K' -2h_z' & -h_x' & -h_x' & -2DA' \\
-h_x' & K' & -2DS' & -h_x' \\
-h_x' & -2DS' & K' & -h_x' \\
-2DA' & -h_x' & -h_x' & -K' + 2h_z'
\end{pmatrix} \quad (2-44) \]

in terms of six independent matrix elements. We will identify the renormalized parameters by comparing this form directly with that of the decimated Hamiltonian.

**Four spin cluster.** The original Hamiltonian for four spins with anisotropic and alternating couplings is
\[
H_b = -K_1(\sigma_0^z\sigma_1^z+\sigma_2^z\sigma_3^z) - DS_1/2 (\sigma_0^+\sigma_1^-+\sigma_2^+\sigma_3^-+h.c) -
- DA_1/2 (\sigma_0^+\sigma_1^-+\sigma_2^+\sigma_3^-+h.c) - K_2\sigma_1^z\sigma_2^z -
- DS_2/2 (\sigma_1^+\sigma_2^-+\sigma_1^-\sigma_2^+) - DA_2/2 (\sigma_1^+\sigma_2^+\sigma_1^-\sigma_2^-) -
- h_z(\sigma_1^z+\sigma_2^z) - h_x/2 (\sigma_1^+\sigma_2^+h.c) -
- h_z\sigma_1(\sigma_0^z+\sigma_3^z) - h_x1/2 (\sigma_0^+\sigma_3^+h.c)
\]

We have allowed the fields on the end spins to be different from those on intermediate spins.

Using the following basis

\[
|1\rangle = |++++\rangle
|2\rangle = |+++\rangle
|3\rangle = |++\rangle
|4\rangle = |+\rangle
|5\rangle = |\rangle
|6\rangle = |\rangle
|7\rangle = |\rangle
|8\rangle = |\rangle
|9\rangle = |+++\rangle
|10\rangle = |+++\rangle
|11\rangle = |++\rangle
|12\rangle = |+\rangle
|13\rangle = |\rangle
|14\rangle = |\rangle
|15\rangle = |\rangle
|16\rangle = |\rangle
\] (2-46)
we develop the 16x16 matrix of the Hamiltonian (2-45) by computer, and diagonalize it to get 16 eigenstates \(|m\rangle\) and eigenenergies \(E(m)\), with

\[
|m\rangle = \sum_{n=1}^{16} v(m,n)|n\rangle
\]  

(2-47)

To decimate, one calculates the partial trace

\[
\exp\{ A_1 - H_b'(K', DS', DA', h_z', h_x') \} = \text{Tr}' \exp\{ -H_b(K, DS, DA, a, h_z, h_x) \}
\]  

(2-48)

In the left side of Eq. (2-48), \(H_b'\) is a 4x4 symmetric matrix that has the form Eq. (2-44). In the right side of Eq. (2-48) \(e^{-H}\) is a 16x16 matrix of the form

\[
\exp\{ -H_b \} = \sum_{m=1}^{16} \exp\{ -E_m \}|m\rangle\langle m|
\]

The trace operation then has the form

\[
\text{Tr}' \; |a_1 A\uparrow + a_2 A\uparrow + a_3 A\uparrow + a_4 A\uparrow\rangle \langle a_1 A\uparrow + a_2 A\uparrow + a_3 A\uparrow + a_4 A\uparrow|
\]

\[
= \left( \sum_{i=1}^{4} a_i |i\rangle \right) \left( \sum_{j=1}^{4} a_j |j\rangle \right) =
\]

\[
\begin{vmatrix}
a_1^2 & a_1a_2 & a_1a_3 & a_1a_4 \\
a_2a_1 & a_2^2 & a_2a_3 & a_2a_4 \\
a_3a_1 & a_3a_2 & a_3^2 & a_3a_4 \\
a_4a_1 & a_4a_2 & a_4a_3 & a_4^2
\end{vmatrix}
\]
where the $|A\rangle$ represents any configuration of the two middle spins, and $|1\rangle$, $|2\rangle$, $|3\rangle$ and $|4\rangle$ are the basis vectors of Eq(2-43). Accordingly we find for right side of Eq.(2-48)

$$\text{Tr} \exp(-H_b) = \sum_{m=1}^{16} \exp(-E_m)$$

Here the matrix elements can be expressed in terms of the expansion coefficients $v(i,j)$:

$$a(1,m) = v_2(1,m) + v_2(2,m) + v_2(9,m) + v_2(10,m)$$
$$a(2,m) = v_2(5,m) + v_2(6,m) + v_2(13,m) + v_2(14,m)$$
$$a(3,m) = v_2(3,m) + v_2(4,m) + v_2(11,m) + v_2(12,m)$$
$$a(4,m) = v_2(7,m) + v_2(8,m) + v_2(15,m) + v_2(16,m)$$
$$a(5,m) = v(1,m) v(5,m) + v(2,m) v(6,m) + v(9,m) v(13,m) + v(10,m) v(14,m)$$
$$a(6,m) = v(1,m) v(3,m) + v(2,m) v(4,m) + v(9,m) v(11,m) + v(10,m) v(12,m)$$
$$a(7,m) = v(1,m) v(7,m) + v(2,m) v(8,m) + v(9,m) v(15,m) + v(10,m) v(16,m)$$
$$a(8,m) = v(5,m) v(3,m) + v(6,m) v(4,m) + v(13,m) v(11,m) + v(14,m) v(12,m)$$
\[ a(9,m)=v(5,m)v(7,m)+v(6,m)v(8,m)+v(13,m)v(15,m)+v(14,m)v(16,m) \]
\[ a(10,m)=v(3,m)v(7,m)+v(4,m)v(8,m)+v(11,m)v(15,m)+v(12,m)v(16,m) \]

Substituting Eq. (2-49) into Eq. (2-48) yields

\[
A_1 - H_{b'} = \ln \sum_{m=1}^{16} e^{-E_m} \begin{bmatrix}
  a(1,m) & a(5,m) & a(6,m) & a(7,m) \\
  a(5,m) & a(2,m) & a(8,m) & a(9,m) \\
  a(6,m) & a(8,m) & a(3,m) & a(10,m) \\
  a(7,m) & a(9,m) & a(10,m) & a(4,m)
\end{bmatrix} = B
\]

(2-50)

We have taken the logarithm of the symmetric matrix by formula Eq. (2-38).

Since the \( H_{b'} \) has form Eq. (2-43), it has zero trace, and we may find directly the spin-independent term which arises from renormalization:

\[
A_1 = \left( \frac{1}{4} \right) \text{Tr} B
\]

(2-51)

We then examine the matrix \( B - \left( \frac{1}{4} \right) (\text{Tr} B) I \) (\( I \) is a 4x4 unit matrix) which has six independent elements

\[
B - \left( \frac{1}{4} \right) (\text{Tr} B) I = \begin{bmatrix}
  A(1) & A(4) & A(4) & A(5) \\
  A(4) & A(2) & A(6) & A(4) \\
  A(4) & A(6) & A(2) & A(4) \\
  A(5) & A(4) & A(4) & A(3)
\end{bmatrix}
\]

(2-52)
From Eqs. 2-44, 50, 51 and 52 we find the renormalized parameters:

\[ K' = -A(2) \]
\[ D_S' = A(6)/2 \]
\[ D_A' = A(5)/2 \] (2-53)
\[ h_z' = (A(1)+A(2))/2 \]
\[ h_x' = A(4) \]

Thermodynamic calculations: The free energy is calculated using the rescaling approach of Eq. (2-33) and the parallel and perpendicular susceptibilities by Eq. (2-25). As a check on our approach, we have calculated the susceptibility for the isotropic antiferromagnetic Heisenberg chain by applying the field in both Z and X directions, and have found no dependence on the field direction (the curve is the same as in Fig. 14). The RG result was also compared with the finite chain data [18]. We have found that at low temperature our L=3 RG result is nearly the same as the four-spin chain result, but with increasing temperature the RG curve approaches the N \( \to \) extrapolation much more rapidly.

For the Ising case, we have compared our results with those of Katsura [14, 59] (see Fig. 23). Our parallel susceptibility is of course exact. For the perpendicular susceptibility, i.e. for the transverse Ising chain, our
result has the right characteristic features, but at low temperature is somewhat larger than Katsura's exact expression.

For the XY-chain case, our result for field in the Z-direction is compared in Fig. 24 with Katsura's exact calculation. The RG result has substantial deviation from the correct curve at low temperature, but the agreement is good for $k_B T/J > 1.0$. In fact it closely approximates Katsura's 6-spin finite chain result. Also shown in Fig. 24 is the susceptibility in the X-direction, for which no exact results are available for comparison.

For the anisotropic case, we must distinguish between perpendicular and parallel susceptibilities. In the case of the uniform and alternating XY-chains, the susceptibilities vs field in the Z- and X-directions, ($\chi_Z$ and $\chi_X$), have been calculated as shown in Fig. 25 and 26. For the alternating XY chain, the double-peaked structure of the alternating isotropic case is evident in both responses, but the maxima for $\chi_X$ are shifted to higher field and there appear as well a number of narrow but distinct peaks, or branches, as compared with those of $\chi_Z$. A double peak arises from the gap that should exist only in alternating cases. Therefore the susceptibilities of uniform chains should have a single peak only. In Fig. 27, at higher temperature we see that only a single peak appears. We
conclude that the small peaks at low temperature arise from the effect of finite clusters. We note that $\mathcal{X}$ shows similar behavior.

These apparently spurious branches constitute a serious problem for the calculation at low temperature. Even at the higher temperature of $k_BT=0.08$ or 0.4, the problem still persists to some degree. To shed some light on this problem, we have checked the iteration sequence for the free energy calculation and the lowest energy levels as functions of field. We have found that the iteration sequences are stable except in the branch areas. In the branch area, points in parameter space which are initially very close together will, under iteration, move to widely separated fixed points —that is, the branch area is a nearly singular region of the flow diagram of the decimation RG. The approximations (neglected commutators) made at each step in the iteration have the effect of switching the system from one RG trajectory to another, and render the results unstable.

If the singular area is small, we may smooth the data by fitting a moderate number of adjacent points to a polynomial of low degree. For the temperatures $k_BT=0.05$, 0.08 and 0.4, we show in Fig. 27 the results of fitting each groups of 10 adjacent points with a cubic. We can see that this procedure reduces the sizes of the branches, but
cannot remove them.

The lowest energy levels of uniform XY-chain have been displayed as functions of field in Fig. 28 and 29. With the field along the Z axis (Fig. 28), the levels are linear functions of $h$. The first ground state crossing point occurs at $H/J=0.61$ and the second at $H/J=1.61$. These correspond roughly to the first and last maxima in the susceptibility picture. When the field is along the X-axis (see Fig. 29), the levels are nonlinear functions of $h$. The first ground state crossing point appears at $H/J=0.97$ and the second at $H/J=2.5$, displacing the peaks to higher field.
Fig. 23. Susceptibility versus temperature for antiferromagnetic Ising chain: the parallel susceptibility lines by $L=3$ RG and by Katsura [14] are same, the perpendicular susceptibility lines by $L=3$ RG and by Katsura are different.
Fig. 24. Susceptibility versus temperature for XY chain. Solid line: line by L=3 RG in x direction field, line by L=3 RG in z direction field, dashed line: Katsura's perpendicular susceptibility line [14]
\[ \alpha = 1. \]

**Fig. 25. Susceptibility vs. magnetic field for uniform XY chain at temperature \( k_B T = 0.05 \). \( \chi_x \) is susceptibility in x direction and \( \chi_z \) is that in the z direction, both by L=3 RG.**
Fig. 26. Susceptibility versus magnetic field for alternating XY chain $\alpha = 0.3$ at temperature $k_B T/J = 0.05$. $\chi_x$ is susceptibility in $x$ direction, and $\chi_z^B$ is that in $z$ direction, both by $L=3$ RG.
Fig. 27. Susceptibility versus x-direction field for uniform XY-chain at different temperature using polynomial fit to each 10 adjacent data points.
Fig. 28. Eight lowest energy levels of uniform XY cluster of four spins as a function of field in the z direction.
Fig. 29. Eight lowest energy levels of uniform XY cluster of 4 spins as a function of field in the x direction.
We have extended the quantum decimation RG:

$$\exp\{ A_1 - H_b' \} = \text{Tr}' \exp\{ -H_b \}$$ (3-1)

to a variety of spin chains, in order to calculate both magnetic and thermal response functions. From a technical point of view three types of situations are encountered in carrying out the RG method:

1. For simple cases, the exact eigenfunctions and eigenvalues of both $H_b'$ and $H_b$ may be found analytically, for instance in the case of the Heisenberg chain in longitudinal field, using a 3-spin cluster. The renormalization transformations may then be found in closed form.

2. $H_b'$ may have eigenfunctions and eigenvalues which can be written in closed form (as in the general free-end cluster and 6-spin ring cases), but the eigenfunctions and eigenvalues of $H_b$ must be found numerically. The decimation procedure is carried out by computer.

3. If the eigenfunctions and eigenvalues of $H_b'$ cannot be found analytically, (for example, the Heisenberg chain with arbitrary field), we must choose a suitable basis in which to represent $H_b'$. The r.h.s of Eq.(3-1) must
then be expressed in the same form as that of the l.h.s., and the decimation procedure can be performed.

In any case, both sides of Eq. (3-1) must be of the same form with the same number of independent terms as unknowns. The decimation (Eq. (3-1)) can then be carried out. We can see that the decimation QRG is flexible and can suit very general situations.

The main approximation in this approach is that non-zero commutators between operators referred to neighboring clusters are ignored. When we increase the size of a cluster the approximation becomes better, in the sense of increasing accuracy at low temperature. We have performed RG calculations using a sequence of spatial scale factors (L=3, 5 and 7) and have noted a clear improvement in those cases in which comparison with finite chain extrapolations are possible.

For the ring decimation case, a bond-moving type of approximation is applied, after which all commutators are accounted for. Comparing the results obtained by N=6 spin ring decimation and those found by L=5 free-end decimation (same number of spins) for the temperature region k_B T/J > 0.8 we find the ring calculations to be more accurate (see Fig. 9 and 10). For the alternating chain case, the ring decimation also gives better critical field values than those found by free-end decimation.
The free energy is found by iterating the decimation procedure. We have used two different iteration techniques (blocking methods) to calculate thermodynamic properties. The second approach (Eq. (2–33)) is designed specifically for chains with alternating interactions, since it converts a uniform chain into an alternating one by the second iteration. Its principal advantage is reduced computer time.

As do all real-space renormalization group methods, the decimation QRG attempts to extract the properties of an infinite system from those of finite-sized clusters. In this respect it is analogous to the process of direct extrapolation of finite-chain calculations. The latter approach is considered to be the most accurate numerical technique available to date, provided it can be extended to reasonably large (~10–12 spins) chains, and we have used its results as a standard for comparison when appropriate. Nevertheless, it can be size-limited, such as in the cases in which the field direction is not longitudinal. In such instances the decimation QRG is particularly useful, since in comparing results for the same size cluster (say 4-spin chain and L=3 RG) we see that the QRG in general is more accurate. The simple finite chain calculation takes into account the eigenvalues, but the QRG uses the eigenfunctions as well.
The other main advantage of the decimation QRG method is that its accuracy improves in the presence of a magnetic field. Thus the decimation QRG is a logical choice for calculating magnetic properties in nonzero field.

The decimation QRG is subject to a number of limitations and technical problems, which we discuss next.

In general, increasing the scale factor L improves the accuracy. At low temperature, however, the three sets of data (L=3, 5 and 7) are not sufficient even for a rough extrapolation.

A more serious difficulty is the fact that the numerical derivatives of the free energy at low temperature appear to be unstable in certain circumstances — particularly in the alternating chain at high field. In these regimes the results depend strongly on the successive points at which the free energy is evaluated. We interpret this behavior as being due to the fact that the true RG trajectories near such points in parameter space are 'closely packed', so that any small change in parameters has a large effect on the results. The QRG involves an approximation (the neglect of certain commutators) at each iteration, whose exact size and effect is difficult to estimate, although we know that it is larger the lower the temperature. At each iteration, then, the renormalized system shifts from one RG trajectory to another, and the net effect can be very irregular at low temperature.
Since these difficulties appear to be related to the fact that the decimation QRG is a high-temperature approximation, we next discuss the possibility of applying a block QRG (see Chapter 1) at high field. The block QRG is more suitable for the zero temperature case, since it preserves the ground and the lowest excited states of the system. However extending the block QRG to high field cases other than the Ising chain in transverse field is still a difficult problem. The transverse Ising chain is the simplest quantum model and is the only spin chain that has been treated by the block QRG in a magnetic field. This is because at any field strength the lowest energy levels of two-spin cluster can map to the energy levels of a single spin (see Fig. 30). On the other hand, the two-spin cluster of the anisotropic Heisenberg chain in longitudinal field has an energy level structure which is difficult to map to the energy levels of a single spin (see Fig. 31). If one uses the even and odd spin block QRG, the energy levels will cross each other as the field is increased (see Fig. 32, say). Therefore the energy levels are too complex to build a suitable mapping relation for all field ranges. On the contrary, the decimation QRG can easily treat the field cases, but it does not work well at low temperature since it does not preserve, in general, the ground state of the system [42].
Fig. 30. Schematic energy levels of transverse Ising model and its block QRG, (a) for 2-spin cluster, (b) for one spin.

Fig. 31. Schematic energy levels of 2-spin cluster for the anisotropic Heisenberg spin chain in the longitudinal field: 1. for the isotropic Heisenberg spin chain, 2. for the XY-like spin chain, 3. for the Ising-like spin chain.
Fig. 32. Schematic energy level structure of isotropic Heisenberg spin cluster: (a) for 3-spin cluster, (b) for 4-spin cluster.
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[11] L. Hulthen, Ark. Mat. Astron. Fys. 26A, no.11 (1938). Here the exchange Hamiltonian used by Hulthen is $-2JS_iS_{i+1}$. Therefore the $J$ is twice as that in Eq.(1-1).


The Hamiltonian in [49] is
\[ \mathcal{H} = - \sum 2J_1(\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} + a \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1}) \]
They found \( J_1/k_B = -2.58K \). Comparing this Hamiltonian with ours Eq (2-26) we find \( K_1 = J_1/(2k_BT) \), e.g. \( K_1 T = -1.29K \).


In order to compare our results with Bonner's results we should change the unit as follows:

The Hamiltonian that Bonner used is
\[ \mathcal{H}_B = -2J_B \sum \mathbf{S}_i \cdot \mathbf{S}_j - H g \mu \sum S_i^z \]
and the Hamiltonian used by us is
\[ \mathcal{H} = -J \sum \mathbf{\sigma}_i \cdot \mathbf{\sigma}_j - H \sum \sigma_i^z \]
here \( S = (1/2)e \). Comparing this, we got
\[ J_B = 2J, \quad \chi_B/(g^2\mu^2) = (1/4)\chi, \quad \mu H_B/J_B = H/J, \]
here \( \chi \) is susceptibility and the quantities that have sub B are used by Bonner.

We use the linear extrapolation method that was used by Bonner and Blöte [52] to estimate the \( L = \infty \) lower critical field values. We assume that the \( h_{c1} \) is smooth function of \( L \):
\[ h_{c1} = a_0 + a_1/L + a_2/L^2. \]
Thus \( a_0 \) is the estimated \( L = \infty \) lower critical field.
In order to compare our results with Katsura's results, we should change the unit as follows: The Hamiltonian that Katsura used is

$$\mathcal{H}_K = -(1/2) \sum J_K \sigma_i \sigma_j - m_H \sum \sigma_i^2$$

Compared with the Hamiltonian that Bonner used [57], we got

$$J_K = J_B, \quad 2m = \sigma \beta \quad \text{and} \quad J_K X_B / (4N \beta^2) = J_B X_B / [(\sigma \beta)^2 N],$$

where the quantities that have sub $K$ are used by Katsura.